From Correlation Functions to Hydrodynamic Behaviour

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Foreword

This is the write-up of my study on this subject in about a 2-month period, as a term paper project for 8.512 *Theory of Solids*. Basically I followed the classic work of L. P. Kadanoff and P. C. Martin in *Annals of Physics* **24**, 419 (1963) and a monograph *Measurements and Correlation Functions* given by P. C. Martin at the Spring School of Ravello (1963). Also J. P. Hanson and I. R. McDonald's book *Theory of Simple Liquids* served as a general reference. I had planned to include the basic formulation of memory functions in this paper, but now it seems to be impossible. One thing I'm always afraid of is that the over-ebullience of formulas will drown the interest of any possible reader and it would seem that I'm simply copying down equations from Kadanoff's paper. Maybe that's true. But I'll strive to explain things in my own ways and fill in derivations that they (ah! the great minds) had regarded as straightforward. At least it had been a tremendous learning experience for myself.

• Mathematical Convention

1. We define the spatial and temporal Fourier transform of a field $M(\mathbf{r}t)$ by

$$M(\mathbf{k}\omega) = \int dt \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega t} M(\mathbf{r}t) \tag{1}$$

when it exists, and the inverse transform

$$M(\mathbf{r}t) = \int \frac{d\omega}{2\pi} \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} M(\mathbf{k}\omega) \tag{2}$$

Whenever $\int$ appears without sub- or superscript it means from $-\infty$ to $+\infty$. In order to ensure convergence, we had implicitly put a convergence factor $e^{-\varepsilon t}$ at $t > 0$ and $e^{\varepsilon t}$ at $t < 0$ inside the integral. In the end ε is limiting to zero. With such properly defined Fourier transform, we have

$$\begin{array}{ll} 1 \Leftrightarrow 2\pi\delta(\omega) & \int A(t-t')B(t')dt' \Leftrightarrow A(\omega)B(\omega) \\ \frac{d^n A(t)}{dt^n} \Leftrightarrow (-i\omega)^n A(\omega) & 2\pi A(t)B(t) \Leftrightarrow \int A(w-\omega')B(\omega')d\omega' \end{array} \tag{3}$$

2. On the other hand, we define complex Laplace transform to be

$$\tilde{M}(\mathbf{r}z) = \int_0^{+\infty} e^{izt} M(\mathbf{r}t) dt \tag{4}$$

where z lies in upper-half complex plane. It follows that

$$\begin{array}{ll} 1 \Leftrightarrow \frac{1}{-iz} & \int_0^t A(t-t')B(t')dt' \Leftrightarrow \tilde{A}(z)\tilde{B}(z) \\ \frac{d^n}{dt^n}A(t) \Leftrightarrow (-iz)^n\tilde{A}(z) - (-iz)^{n-1}A(t=0) - (-iz)^{n-2}A'(t=0) - \ldots & \end{array} \tag{5}$$

By $\tilde{M}(\mathbf{r}\omega)$ we mean

$$\tilde{M}(\mathbf{r}\omega) = \lim_{\varepsilon\to 0^+} \tilde{M}(\mathbf{r}, w + i\varepsilon) \tag{6}$$

If $M(\mathbf{r}t) = 0$ for $t < 0$, then $M(\mathbf{r}\omega) = \tilde{M}(\mathbf{r}\omega)$, and as a convention we'll always omit the tilde on $\tilde{M}(\mathbf{r}z)$.

3. The relationship between $\tilde{M}(\mathbf{r}z)$ and $M(\mathbf{r}\omega)$, if $M(\mathbf{r}\omega)$ exists, is

$$\begin{aligned} \tilde{M}(\mathbf{r}z) \quad &= \int_0^{+\infty} e^{izt} M(\mathbf{r}t)dt \\ &= \int_0^{+\infty} e^{izt} \int \frac{d\omega}{2\pi} e^{-i\omega t} M(\mathbf{r}\omega) \\ &= \int \frac{d\omega}{2\pi i} \frac{M(\mathbf{r}\omega)}{\omega - z} \end{aligned} \tag{7}$$

4. The "well-known formula of complex algebra":

$$\lim_{\varepsilon\to 0^+} \frac{1}{x + i\varepsilon} = \mathcal{P}\frac{1}{x} - i\pi\delta\left(x\right) \tag{8}$$

where $\mathcal{P}$ means principle part integration, which enable it to bypass certain singularities. We also have

$$\lim_{\varepsilon\to 0^+} \frac{\varepsilon}{x^2 + \varepsilon^2} = \pi\delta\left(x\right) \tag{9}$$

5. If a response function $\chi(\mathbf{r}t) = \chi(\mathbf{r}t)\eta(t)$ ($\eta(t)$ is the Heaviside step-function), i.e., $X(\mathbf{r}, t < 0) = 0$, then it's *causal* and $\chi(\mathbf{r}\omega) = \tilde{\chi}(\mathbf{r}\omega)$ and we always omit the tilde on $\tilde{\chi}(\mathbf{r}z)$. It then can be shown (8.512 PS #3.1) that Kramers-Kronig relations apply:

$$\chi(\mathbf{r}z) = \int \frac{d\omega'}{\pi} \frac{\mathrm{Im}\chi(\mathbf{r}\omega')}{\omega' - z} = \int \frac{d\omega'}{\pi i} \frac{\mathrm{Re}\chi(\mathbf{r}\omega')}{\omega' - z} \tag{10}$$

and

$$\mathrm{Re}\chi(\mathbf{r}\omega) = \mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Im}\chi(\mathbf{r}\omega')}{\omega' - \omega} \tag{11}$$

$$\mathrm{Im}\chi(\mathbf{r}\omega) = -\mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Re}\chi(\mathbf{r}\omega')}{\omega' - \omega} \tag{12}$$

Chapter 1

Linear Response and Properties of Dynamic Susceptibility

Suppose under the original time-independent Hamiltonian $\mathcal{H}_0$ the time-evolution operator is $U_0(t) = \exp\left(-i\mathcal{H}_0 t/\hbar\right)$, then after we add in time-dependent perturbation $V(t)$ it changes to $U(t)$, which satisfies Schrodinger's equation

$$i\hbar\frac{\partial}{\partial t}U(t) = (\mathcal{H}_0 + V(t))U(t) \tag{1.1}$$

If we define

$$U(t) = U_0(t)U_I(t) \tag{1.2}$$

and

$$\mathcal{H}_I(t) = e^{i\mathcal{H}_0 t/\hbar}V(t)e^{-i\mathcal{H}_0 t/\hbar} \tag{1.3}$$

where subscript I denotes "interaction picture". It's easy to show that

$$i\hbar\frac{\partial}{\partial t}U_I(t) = \mathcal{H}_I(t)U_I(t) \tag{1.4}$$

and so, by iteration

$$\begin{aligned} U_I(t) \quad &= 1 - \frac{i}{\hbar}\int_0^t \mathcal{H}_I(t')dt' + (-\frac{i}{\hbar})^2\int_0^t \mathcal{H}_I(t')dt'\int_0^{t'}\mathcal{H}_I(t'')dt'' + ... \\ &= T\exp\left(-\frac{i}{\hbar}\int_0^t \mathcal{H}_I(t')dt'\right) \end{aligned} \tag{1.5}$$

Notice that the so-called "interaction picture" is relative to the current *perturbed* Hamiltonian, but actually it's also Heisenberg operator to the original unperturbed Hamiltonian. It is this aspect that links the behaviour of perturbed system to its equilibrium behaviour.

Suppose at $t = 0$ the system is at state $|\alpha\rangle$ with no perturbation. After $t > 0$ the perturbation is turned on. For any dynamical variable A, its measurement at $t > 0$ is

$$\begin{aligned}\langle A(t)\rangle_{n.e.} &= \langle\alpha|U^\dagger(t)AU(t)|\alpha\rangle \\ &= \langle\alpha|U_I^\dagger(t)U_0^\dagger(t)AU_0(t)U_I(t)|\alpha\rangle \\ &= \langle\alpha|U_I^\dagger(t)A_I(t)U_I(t)|\alpha\rangle \qquad (1.6)\end{aligned}$$

To linear order $U_I(t)$ could be expanded by virtue of Eqn(1.5) in terms of $\mathcal{H}_I(t)$, then

$$\begin{aligned}\langle A(t)\rangle_{n.e.} &= \langle\alpha|\Big(1 + \frac{i}{\hbar}\int_0^t \mathcal{H}_I(t')dt'\Big)A_I(t)\Big(1 - \frac{i}{\hbar}\int_0^t \mathcal{H}_I(t')dt'\Big)|\alpha\rangle + \mathcal{O}(\mathcal{H}_I^2) \\ &= \langle\alpha|A_I(t)|\alpha\rangle - \frac{i}{\hbar}\int_0^t \langle\alpha|[A_I(t), \mathcal{H}_I(t')]|\alpha\rangle dt' + \mathcal{O}(\mathcal{H}_I^2) \qquad (1.7)\end{aligned}$$

From now on I'll omit subscript I and replace $\langle\alpha| \quad |\alpha\rangle$ by $\langle\ \rangle$, the equilibrium ensemble average (for finite temperature systems $|\alpha\rangle$'s will be averaged over with proper weight), and define

$$\delta\langle A(t)\rangle = \langle A(t)\rangle_{n.e.} - \langle A(t)\rangle \qquad (1.8)$$

the net response of $\langle A(t)\rangle$ to the perturbation.

At this point we introduce field variables as we want to study both temporal and spatial correlations. For instance, $A(t)$ can be $n(\mathbf{r}t)$, the particle density operator at $\mathbf{r}$

$$n(\mathbf{r}t) = \sum_i \delta\left(\mathbf{r} - \mathbf{r}_i(t)\right) \qquad (1.9)$$

There exist constitutive relations for these QM operators just as in the classical case: for Heisenberg operators with no explicit time depenedence

$$\frac{dA(t)}{dt} = \frac{i}{\hbar}[\mathcal{H}_0, A(t)] \qquad (1.10)$$

and we assume $\mathcal{H}_0$ to be of the form

$$\mathcal{H}_0 = \sum_i \frac{\mathbf{p}_i^2}{2m} + V(\{\mathbf{r}_i\}) \tag{1.11}$$

then

$$\begin{aligned}
\frac{dn(\mathbf{r}t)}{dt} &= \frac{i}{\hbar}[\mathcal{H}_0, \sum_i \delta\left(\mathbf{r}-\mathbf{r}_i(t)\right)] \\
&= \frac{i}{\hbar}[\sum_j \frac{\mathbf{p}_j^2}{2m}, \sum_i \delta\left(\mathbf{r}-\mathbf{r}_i(t)\right)] \\
&= \frac{1}{2m}\sum_i \nabla_i \delta\left(\mathbf{r}-\mathbf{r}_i(t)\right)\cdot\mathbf{p}_i + \mathbf{p}_i\cdot\nabla_i\delta\left(\mathbf{r}-\mathbf{r}_i(t)\right) \\
&= -\nabla\cdot\left(\delta\left(\mathbf{r}-\mathbf{r}_i(t)\right)\frac{\mathbf{p}_i}{2m} + \frac{\mathbf{p}_i}{2m}\delta\left(\mathbf{r}-\mathbf{r}_i(t)\right)\right) \\
&= -\nabla\cdot\mathbf{J}(\mathbf{r}t) \qquad (1.12)
\end{aligned}$$

where $\mathbf{J}(\mathbf{r}t)$ is the particle current operator

$$\mathbf{J}(\mathbf{r}t) = \sum_i \{\mathbf{p}_i/2m, \delta\left(\mathbf{r}-\mathbf{r}_i(t)\right)\} \tag{1.13}$$

Notice the $\mathbf{J}(\mathbf{r}t)$ is written in anticommutator form to ensure Hermiticity. This is in general the case when going from classical to QM expressions. Suppose the perturbation Hamiltonian $V(t)$ can be written in the form

$$V(t) = -\int B(\mathbf{r})f(\mathbf{r}t)dr \tag{1.14}$$

where $B(\mathbf{r})$ is an operator and $f(\mathbf{r}t)$ is a number with the meaning of *force*, then

$$\delta\left\langle A(\mathbf{r}t)\right\rangle = \frac{i}{\hbar}\int_{-\infty}^{t}\langle[A(\mathbf{r}t), B(\mathbf{r}'t')]\rangle f(\mathbf{r}'t')d\mathbf{r}'dt' \tag{1.15}$$

where we allow for perturbation from $-\infty$ to $+\infty$. Let's define

$$\begin{aligned}
\langle[A(\mathbf{r}t), B(\mathbf{r}'t')]\rangle &= 2\hbar\chi''_{AB}(\mathbf{r}\mathbf{r}', t-t') \\
&= 2\hbar\int\frac{d\omega}{2\pi}e^{-i\omega(t-t')}\chi''_{AB}(\mathbf{r}\mathbf{r}', \omega) \qquad (1.16)
\end{aligned}$$

and

$$\chi_{AB}(\mathbf{r}\mathbf{r}', t-t') = 2i\eta(t-t')\chi''_{AB}(\mathbf{r}\mathbf{r}', t-t') \tag{1.17}$$

such that we can get rid of the upper-integration limit t in Eqn(1.15) and write

$$\delta \langle A(\mathbf{r}t)\rangle = \int\int d\mathbf{r}'dt'\chi_{AB}(\mathbf{r}\mathbf{r}', t-t')f(\mathbf{r}'t') \tag{1.18}$$

$\chi_{AB}(\mathbf{r}\mathbf{r}', t-t')$ is called the *dynamic susceptibility* or *response function.* $\chi''_{AB}(\mathbf{r}\mathbf{r}', t-t')$ is its *absorptive* or *dissipation* part, the reason of which will be clear very soon. χ''_{AB} has the following properties,

1. Since both A and B are Hermitian

   $$[A(\mathbf{r}t), B(\mathbf{r}'t')]^\dagger = -[A(\mathbf{r}t), B(\mathbf{r}'t')] \tag{1.19}$$

   so $\chi''_{AB}(\mathbf{r}\mathbf{r}', t-t')$ must be imaginary

   $$\chi''^{*}_{AB}(\mathbf{r}\mathbf{r}', t-t') = -\chi''_{AB}(\mathbf{r}\mathbf{r}', t-t') \qquad \chi''^{*}_{AB}(\mathbf{r}\mathbf{r}', -\omega) = -\chi''_{AB}(\mathbf{r}\mathbf{r}', \omega) \tag{1.20}$$

   Also because it's a commutator

   $$\chi''_{AB}(\mathbf{r}\mathbf{r}', t-t') = -\chi''_{BA}(\mathbf{r}'\mathbf{r}, t'-t) \tag{1.21}$$

2. Usually A, B are operators with definite "signiture" ±1 under time-reversal operator $K = -i\sigma_y C$

   $$KAK^{-1} = \varepsilon_A A \qquad KBK^{-1} = \varepsilon_B B \qquad (\varepsilon_A, \varepsilon_B = \pm 1) \tag{1.22}$$

   And so is the initial state $|\alpha\rangle$ if the unperturbed Hamiltonian $\mathcal{H}_0$ commutes with $K, K|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle$. Then

   $$\begin{aligned}\langle\alpha|[A(\mathbf{r}t), B(\mathbf{r}'t')]|\alpha\rangle &= \Big(|\alpha\rangle, [A(\mathbf{r}t), B(\mathbf{r}'t')]|\alpha\rangle\Big) \\ &= \Big(K[A(\mathbf{r}t), B(\mathbf{r}'t')]|\alpha\rangle, K|\alpha\rangle\Big) \\ &= \Big(K[A(\mathbf{r}t), B(\mathbf{r}'t')]K^{-1}K|\alpha\rangle, K|\alpha\rangle\Big) \\ &= \varepsilon_\alpha^2\varepsilon_A\varepsilon_B\Big([A(\mathbf{r}, -t), B(\mathbf{r}', -t')]|\alpha\rangle, |\alpha\rangle\Big) \\ &= -\varepsilon_A\varepsilon_B\Big(|\alpha\rangle, [A(\mathbf{r}, -t), B(\mathbf{r}', -t')]|\alpha\rangle\Big) \qquad (1.23)\end{aligned}$$

so

$$\chi''_{AB}(\mathbf{rr}', t-t') = -\varepsilon_A\varepsilon_B\chi''_{AB}(\mathbf{rr}', t'-t) \tag{1.24}$$

Combined with 1, there are two possibilities

(a)

$$\begin{aligned}\varepsilon_A = \varepsilon_B: \;\; &\chi''_{AB}(\mathbf{rr}', t-t') = -\chi''_{AB}(\mathbf{rr}', t'-t) = \chi''_{BA}(\mathbf{r}'\mathbf{r}, t-t') \\ &\chi''_{AB}(\mathbf{rr}', \omega) \text{ is real and odd}\end{aligned} \tag{1.25}$$

(b)

$$\begin{aligned}\varepsilon_A = -\varepsilon_B: \;\; &\chi''_{AB}(\mathbf{rr}', t-t') = \chi''_{AB}(\mathbf{rr}', t'-t) = -\chi''_{BA}(\mathbf{r}'\mathbf{r}, t-t') \\ &\chi''_{AB}(\mathbf{rr}', \omega) \text{ is imaginary and even}\end{aligned} \tag{1.26}$$

Now since $\chi_{AB}(\mathbf{rr}', t-t')$ is causal, we have the analytic continued Fourier transform

$$\begin{aligned}\chi_{AB}(\mathbf{rr}', z) = &\int_{-\infty}^{+\infty} e^{izt} 2i\eta(t)\chi''_{AB}(\mathbf{rr}', t)dt \\ = &\int_{0}^{+\infty} e^{izt} 2i \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} e^{-i\omega' t}\chi''_{AB}(\mathbf{rr}', \omega')dt \\ = &\int_{-\infty}^{+\infty} \frac{d\omega'}{\pi}\frac{\chi''_{AB}(\mathbf{rr}', \omega')}{\omega' - z}\end{aligned} \tag{1.27}$$

with z in the upper-half complex plane. We then have

$$\begin{aligned}\chi_{AB}(\mathbf{rr}', \omega) = &\lim_{\varepsilon\to 0^+} \chi_{AB}(\mathbf{rr}', z = \omega + i\varepsilon) \\ = &\int_{-\infty}^{+\infty} \frac{d\omega'}{\pi}\frac{\chi''_{AB}(\mathbf{rr}', \omega')}{\omega' - \omega - i\varepsilon} \\ = &\mathcal{P}\int_{-\infty}^{+\infty} \frac{d\omega'}{\pi}\frac{\chi''_{AB}(\mathbf{rr}', \omega')}{\omega' - \omega} + i\chi''_{AB}(\mathbf{rr}', \omega)\end{aligned} \tag{1.28}$$

It's convienient now to define

$$\chi'_{AB}(\mathbf{rr}', \omega) = \mathcal{P}\int_{-\infty}^{+\infty} \frac{d\omega'}{\pi}\frac{\chi''_{AB}(\mathbf{rr}', \omega')}{\omega' - \omega} \tag{1.29}$$

and then there is

$$\chi_{AB}(\mathbf{rr}', \omega) = \chi'_{AB}(\mathbf{rr}', \omega) + i\chi''_{AB}(\mathbf{rr}', \omega) \tag{1.30}$$

We often call χ'_{AB} and χ''_{AB} the *real* and *imaginary* part of the dynamic susceptibility by reason of the above equation. But keep in mind that it's only true when $\varepsilon_A = \varepsilon_B$ so

$\chi''_{AB}(\mathbf{rr}',\omega)$ and $\chi'_{AB}(\mathbf{rr}',\omega)$ are then real, in which case $\chi'_{AB}(\mathbf{rr}',\omega)$ would be an even function of ω. On the other hand, irrespective of whether this is true, i.e., whether $\chi''_{AB}(\mathbf{rr}',\omega)$ is the real or imaginary part of $\chi_{AB}(\mathbf{rr}',\omega)$ (must be one), from the Kramers-Kronig relations Eqn(11),Eqn(12) for causal systems the following identity always hold

$$\chi''_{AB}(\mathbf{rr}',\omega) = -\mathcal{P}\int \frac{d\omega'}{\pi}\frac{\chi'_{AB}(\mathbf{rr}',\omega')}{\omega'-\omega} \tag{1.31}$$

- **Sum rules in terms of equal-time commutators**

Since

$$\begin{aligned}\langle [A(\mathbf{r}t), B(\mathbf{r}'t')]\rangle = & \quad 2\hbar\chi''_{AB}(\mathbf{rr}',t-t') \\ = & \quad 2\hbar\int\frac{d\omega}{2\pi}e^{-i\omega(t-t')}\chi''_{AB}(\mathbf{rr}',\omega)\end{aligned} \tag{1.32}$$

$$\left\langle [(i\frac{d}{dt})^n A(\mathbf{r}t), B(\mathbf{r}'t)]\right\rangle = 2\hbar\int\frac{d\omega}{2\pi}\omega^n\chi''_{AB}(\mathbf{rr}',\omega) \tag{1.33}$$

by letting $t' = t$ after taking the derivative. Equivalently

$$\frac{1}{\hbar}\langle[[[A(\mathbf{r}t),\mathcal{H}_0/\hbar],...,\mathcal{H}_0/\hbar],B(\mathbf{r}'t)]\rangle = \int\frac{d\omega}{\pi}\omega^n\chi''_{AB}(\mathbf{rr}',\omega) \tag{1.34}$$

The LHS of the equation, at least for the first few terms, could be calculated theoretically once the model is known. Thus we obtains exact *sum rules* or *moment expansions* for $\chi''_{AB}(\mathbf{rr}',\omega)$ which, when combined with the hydrodynamic behaviours at low frequencies, could provide us a fitting scheme for χ''_{AB} (the memory function is a formalism to provide physical meaning to this activity). Some famous sum rules will be introduced in later examples.

- **Links of χ''_{BB} with dissipation**

Under the Hamiltonian

$$\mathcal{H}(t) = \mathcal{H}_0 - \int d\mathbf{r}B(\mathbf{r})f(\mathbf{r}t) \tag{1.35}$$

the expectation of system energy $\langle\mathcal{H}(t)\rangle$ would change with time. By the equation of motion for observables

$$\frac{d\langle A(t)\rangle}{dt} = \frac{i}{\hbar}\langle\alpha, t\,|[\mathcal{H}(t), A(t)]|\,\alpha, t\rangle + \langle\alpha, t|\frac{\partial A(t)}{\partial t}|\alpha, t\rangle \tag{1.36}$$

Thus $d\langle\mathcal{H}(t)\rangle/dt$ only depends on the explicit time derivative

$$\begin{aligned}\frac{d\langle\mathcal{H}(t)\rangle}{dt} &= \quad \langle\alpha, t| - \int d\mathbf{r}B(\mathbf{r})\frac{df(\mathbf{r}t)}{dt}|\alpha, t\rangle \\ &= \quad -\int d\mathbf{r}\dot{f}(\mathbf{r}t)\langle\alpha|B(\mathbf{r}t)|\alpha\rangle \\ &= \quad -\int d\mathbf{r}\dot{f}(\mathbf{r}t)\int\chi_{BB}(\mathbf{r}\mathbf{r}', t-t')f(\mathbf{r}'t')d\mathbf{r}'dt' \end{aligned} \tag{1.37}$$

It's enough to study monochromatic perturbation

$$f(\mathbf{r}t) = \frac{1}{2}[f(\mathbf{r})e^{-i\omega t} + f^*(\mathbf{r})e^{i\omega t}] \tag{1.38}$$

then

$$\begin{aligned}\text{RHS} = \quad & -\frac{1}{4}\int d\mathbf{r}\Big(-i\omega f(\mathbf{r})e^{-i\omega t} + i\omega f^*(\mathbf{r})e^{i\omega t}\Big)\chi_{BB}(\mathbf{r}\mathbf{r}', t-t')\Big(f(\mathbf{r}')e^{-i\omega t'} + f^*(\mathbf{r}')e^{i\omega t'}\Big)d\mathbf{r}'dt' \\ = \quad & -\frac{1}{4}\int d\mathbf{r}d\mathbf{r}'dt'\chi_{BB}(\mathbf{r}\mathbf{r}', t-t')\Big(-i\omega f(\mathbf{r})f^*(\mathbf{r}')(e^{-i\omega(t-t')} - e^{i\omega(t-t')}) \\ & - i\omega f(\mathbf{r})f(\mathbf{r}')e^{-i\omega(t+t')} + i\omega f^*(\mathbf{r})f^*(\mathbf{r}')e^{i\omega(t+t')}\Big) \end{aligned} \tag{1.39}$$

where we had made use of Eqn(1.25) to show that

$$\chi_{BB}(\mathbf{r}\mathbf{r}', t-t') = \chi_{BB}(\mathbf{r}'\mathbf{r}, t-t') \tag{1.40}$$

notice that we do not have to have any spatial symmetry to achieve this reciprocity. We are only interested in components that make steady contribution, so the last two terms vanishes in the long run

$$\overline{\frac{d\langle\mathcal{H}(t)\rangle}{dt}} = \frac{1}{4}\int d\mathbf{r}d\mathbf{r}'i\omega f(\mathbf{r})f^*(\mathbf{r}')(\chi_{BB}(\mathbf{r}\mathbf{r}', -\omega) - \chi_{BB}(\mathbf{r}\mathbf{r}', \omega)) \tag{1.41}$$

Because $\chi'_{BB}(\mathbf{r}\mathbf{r}', \omega)$ is even while $\chi''_{BB}(\mathbf{r}\mathbf{r}', \omega)$ is odd in ω

$$\overline{\frac{d\langle\mathcal{H}(t)\rangle}{dt}} = \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'f(\mathbf{r})f^*(\mathbf{r}')\omega\chi''_{BB}(\mathbf{r}\mathbf{r}', \omega) \tag{1.42}$$

So long as the system is stable, there can be only net dissipation at all frequencies. If the system is translational invariant, then $\chi''_{BB}(\mathbf{r}\mathbf{r}',\omega) = \chi''_{BB}(\mathbf{r}-\mathbf{r}',\omega)$, and Eqn(1.42) become

$$\overline{\frac{d\langle\mathcal{H}(t)\rangle}{dt}} = \frac{1}{2}\int d\mathbf{k}|f(\mathbf{k})|^2\omega\chi''_{BB}(\mathbf{k},\omega) \tag{1.43}$$

so there must be

$$\omega\chi''_{BB}(\mathbf{k}\omega) \geq 0 \tag{1.44}$$

for all $(\mathbf{k},\omega)$. This will be shown to hold for canonical and grand-canonical ensembles in the following chapter by using the fluctuation-dissipation theorem and Lehmann representation. This leads to the conclusion that, from Eqn(1.29), that at small ω, $\chi'(\mathbf{k}\omega)$ must be positive definite. And at large ω

$$\begin{aligned}
\chi'_{BB}(\mathbf{k}\omega) = & \quad \mathcal{P}\int_{-\infty}^{+\infty}\frac{d\omega'}{\pi}\frac{\chi''_{BB}(\mathbf{k}\omega')}{\omega'-\omega} \\
= & \quad \mathcal{P}\int_{-\infty}^{+\infty}\frac{d\omega'}{\pi}\chi''_{BB}(\mathbf{k}\omega')\left(-\frac{1}{\omega}-\frac{\omega'}{\omega^2}+...\right) \\
= & \quad -\frac{1}{\omega^2\pi}\int_{-\infty}^{+\infty}d\omega'\omega'\chi''_{BB}(\mathbf{k}\omega')+... \\
\leq & \quad 0
\end{aligned} \tag{1.45}$$

that's going to be negative definite. This corresponds to the statement that a forced oscillator will be in the direction of the force at low frequencies, while 180° out of phase at high frequencies. On both ends dissipation will be small. Large dissipation will happen at intermediate frequencies, where sometimes *local modes* — infinitely sharp resonances, occur. That corresponds to a spike in $\chi''_{BB}(\mathbf{r}\mathbf{r}',\omega)$. Keep in mind that in these cases usually some lower level response functions play the major role, say, if $\chi_{BB} = \chi_{xx}$, where x is the displacement of some kind of oscillator, then local mode happens when $\chi'_{vv}(\omega)$ goes to zero at places where $\chi''_{vv}(\omega)$ is already zero — v is the velocity. A rule of thumb in the mathematical treatment of this problem is to assume that $\chi''_{vv}(\omega)$ is still a small positive number (absorption peak: $\omega > 0$), which plays the role of ε.

Chapter 2

Fluctuation-Dissipation Theorem and Correlation Functions

In canonical ensemble, the initial states of Eqn(1.15) are averaged over with density matrix $\exp\left(-\beta\mathcal{H}_0\right)/\mathrm{Tr}\exp\left(-\beta\mathcal{H}_0\right)$. Because

$$\begin{aligned}\mathrm{Tr}e^{-\beta\mathcal{H}_0}A(\mathbf{r}t)B(\mathbf{r}'t') = & \quad \mathrm{Tr}e^{-\beta\mathcal{H}_0}e^{i\mathcal{H}_0t/\hbar}A(\mathbf{r})e^{-i\mathcal{H}_0t/\hbar}B(\mathbf{r}'t') \\ = & \quad \mathrm{Tr}e^{i\mathcal{H}_0(t+i\hbar\beta)/\hbar}A(\mathbf{r})e^{-i\mathcal{H}_0(t+i\hbar\beta)/\hbar}e^{-\beta\mathcal{H}_0}B(\mathbf{r}'t') \\ = & \quad \mathrm{Tr}A(\mathbf{r},t+i\hbar\beta)e^{-\beta\mathcal{H}_0}B(\mathbf{r}'t') \\ = & \quad \mathrm{Tr}e^{-\beta\mathcal{H}_0}B(\mathbf{r}'t')A(\mathbf{r},t+i\hbar\beta) \end{aligned} \tag{2.1}$$

so

$$\langle A(\mathbf{r}t)B(\mathbf{r}'t')\rangle = \langle B(\mathbf{r}'t')A(\mathbf{r},t+i\hbar\beta)\rangle \tag{2.2}$$

Also notice that $\langle A(\mathbf{r}t)\rangle$ and $\langle B(\mathbf{r}t)\rangle$ are independent of t under $\mathcal{H}_0$. If we define

$$\begin{aligned} f_{AB}(\mathbf{r}\mathbf{r}',t-t') = & \quad \frac{1}{2}\Big\langle\Big(A(\mathbf{r}t)-\langle A(\mathbf{r})\rangle\Big)\Big(B(\mathbf{r}'t')-\langle B(\mathbf{r}')\rangle\Big)\Big\rangle \\ = & \quad \int\frac{d\omega}{2\pi}f_{AB}(\mathbf{r}\mathbf{r}',\omega)e^{-i\omega(t-t')} \end{aligned} \tag{2.3}$$

(the constant parts $\langle A(\mathbf{r})\rangle, \langle B(\mathbf{r})\rangle$ have to be subtracted from $A(\mathbf{r}t), B(\mathbf{r}t)$ in order for the following time-shifting operation in the complex plane to be valid. Try constant A, B.) then

$$\begin{aligned} f_{AB}(\mathbf{r}\mathbf{r}', \omega) = &\quad \int dt e^{i\omega(t-t')} f_{AB}(\mathbf{r}\mathbf{r}', t-t') \\ = &\quad \int dt e^{i\omega(t-t')} f_{BA}(\mathbf{r}'\mathbf{r}, t'-t-i\hbar\beta) \\ = &\quad \int dt e^{i\omega(t+i\hbar\beta-t')+\beta\hbar\omega} f_{BA}(\mathbf{r}'\mathbf{r}, t'-t-i\hbar\beta) \\ = &\quad e^{\beta\hbar\omega} f_{BA}(\mathbf{r}'\mathbf{r}, -\omega) \end{aligned} \tag{2.4}$$

On the other hand since

$$\begin{aligned} \chi''_{AB}(\mathbf{r}\mathbf{r}', t-t') = &\quad \frac{1}{2\hbar}\langle [A(\mathbf{r}t), B(\mathbf{r}'t')]\rangle \\ = &\quad \frac{1}{2\hbar}\langle [A(\mathbf{r}t) - \langle A(\mathbf{r})\rangle, B(\mathbf{r}'t') - \langle B(\mathbf{r}')\rangle]\rangle \\ = &\quad \frac{1}{\hbar}(f_{AB}(\mathbf{r}\mathbf{r}', t-t') - f_{BA}(\mathbf{r}'\mathbf{r}, t'-t)) \end{aligned} \tag{2.5}$$

So

$$\begin{aligned} \chi''_{AB}(\mathbf{r}\mathbf{r}', \omega) = &\quad \frac{1}{\hbar}(f_{AB}(\mathbf{r}\mathbf{r}', \omega) - f_{BA}(\mathbf{r}'\mathbf{r}, -\omega)) \\ = &\quad \frac{1}{\hbar}(1 - e^{-\beta\hbar\omega}) f_{AB}(\mathbf{r}\mathbf{r}', \omega) \end{aligned} \tag{2.6}$$

Define symmetrized product (or *correlation function*)

$$C_{AB}(\mathbf{r}\mathbf{r}', t-t') = \frac{1}{2}\langle\{A(\mathbf{r}t) - \langle A(\mathbf{r})\rangle, B(\mathbf{r}'t') - \langle B(\mathbf{r}')\rangle\}\rangle \tag{2.7}$$

then following the same procedure

$$C_{AB}(\mathbf{r}\mathbf{r}', \omega) = (1 + e^{-\beta\hbar\omega}) f_{AB}(\mathbf{r}\mathbf{r}', \omega) \tag{2.8}$$

And so

$$C_{AB}(\mathbf{r}\mathbf{r}', \omega) = \hbar\frac{1 + e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}}\chi''_{AB}(\mathbf{r}\mathbf{r}', \omega) = \hbar\coth\frac{\beta\hbar\omega}{2}\chi''_{AB}(\mathbf{r}\mathbf{r}', \omega) \tag{2.9}$$

This relation between the anticommutator and commutator of A and B is called the *fluctuation-dissipation theorem* because C_{AB} describe correlations of spontaneous fluctuations in the equilibrium system, while χ''_{AB} describe the non-equilibrium behaviour of that system due to external perturbation and the ensuing energy dissipation. This theorem is the bridge of going from equilibrium measurables (correlation functions) to its non-equilibrium behaviour. Notice that Eqn(2.9) also holds true for grand-canonical ensembles in exactly the same form if A and B commutes with the number operator N.

As the first application the fluctuation-dissipation theorem, we'll prove the stability of canonical/grand-canonical systems. Consider $C_{BB}(\mathbf{r}\mathbf{r}',\omega)$

$$
\begin{aligned}
&\int d\mathbf{r}d\mathbf{r}' f(\mathbf{r})f^*(\mathbf{r}')C_{BB}(\mathbf{r}\mathbf{r}',\omega) \\
= \quad & \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' f(\mathbf{r})f^*(\mathbf{r}')\int dt e^{i\omega t}\langle\{\delta B(\mathbf{r}t),\delta B(\mathbf{r}'0)\}\rangle \\
= \quad & \frac{1}{2}\int dE\rho_C(E)dE'\rho(E')\int d\mathbf{r}d\mathbf{r}' f(\mathbf{r})f^*(\mathbf{r}')\int dt e^{i\omega t}\Big(\langle E|\delta B(\mathbf{r}t)|E'\rangle\langle E'|\delta B(\mathbf{r}'0)|E\rangle + \\
& \qquad \langle E|\delta B(\mathbf{r}'0)|E'\rangle\langle E'|\delta B(\mathbf{r}t)|E\rangle\Big) \\
= \quad & \frac{1}{2}\int dE\rho_C(E)dE'\rho(E')\int d\mathbf{r}d\mathbf{r}' f(\mathbf{r})f^*(\mathbf{r}')\int dt e^{i(\omega-\frac{E'}{\hbar}+\frac{E}{\hbar})t}\langle E|\delta B(\mathbf{r}0)|E'\rangle\langle E'|\delta B(\mathbf{r}'0)|E\rangle \\
& \qquad + e^{i(\omega+\frac{E'}{\hbar}-\frac{E}{\hbar})t}\langle E|\delta B(\mathbf{r}'0)|E'\rangle\langle E'|\delta B(\mathbf{r}0)|E\rangle \\
= \quad & \frac{1}{2}\int dE\rho_C(E)dE'\rho(E')2\pi[\delta\left(\omega-\frac{E'}{\hbar}+\frac{E}{\hbar}\right)+\delta\left(\omega+\frac{E'}{\hbar}-\frac{E}{\hbar}\right)]\left|\int d\mathbf{r}f(\mathbf{r})\langle E|\delta B(\mathbf{r}0)|E'\rangle\right|^2
\end{aligned}
\tag{2.10}
$$

where $\rho(E')$ is the density of states and $\rho_C(E)$ is the canonical/ grand-canonical weighted one. So, by Eqn(1.42), we have

$$
\begin{aligned}
&\frac{\overline{d\langle\mathcal{H}(t)\rangle}}{dt} \\
= \quad & \frac{\omega}{2}\int d\mathbf{r}d\mathbf{r}' f(\mathbf{r})f^*(\mathbf{r}')\chi''_{BB}(\mathbf{r}\mathbf{r}',\omega) \\
= \quad & \frac{\omega}{2\hbar}\tanh\frac{\beta\hbar\omega}{2}\int d\mathbf{r}d\mathbf{r}' f(\mathbf{r})f^*(\mathbf{r}')C_{BB}(\mathbf{r}\mathbf{r}',\omega) \\
= \quad & \frac{\omega}{4}\tanh\frac{\beta\hbar\omega}{2}\int dE\rho_C(E)dE'\rho(E')2\pi[\delta\left(\hbar\omega-E'+E\right)+\delta\left(\hbar\omega+E'-E\right)] \\
& \qquad \left|\int d\mathbf{r}f(\mathbf{r})\langle E|\delta B(\mathbf{r}0)|E'\rangle\right|^2
\end{aligned}
\tag{2.11}
$$

We see that it must be a positive definite quantity. Also notice its link to Fermi's Golden Rule.

As a second application, we'll prove an identity that's instructive when compared with expressions of classical linear response theory

$$\int_0^{\beta} \left\langle \dot{A}(\mathbf{r}t)B(\mathbf{r}', i\hbar\beta')\right\rangle d\beta' = -\frac{i}{\hbar}\langle [A(\mathbf{r}t), B(\mathbf{r}0)]\rangle \tag{2.12}$$

the $\langle\ \rangle$ is averaged in constant temperature β.

- **Proof:** First notice that because $\langle A(t+t')B(t')\rangle$ is independent t' when $\mathcal{H}_0$ is independent of time

$$\left\langle \dot{A}(\mathbf{r}t)B(\mathbf{r}'0)\right\rangle + \left\langle A(\mathbf{r}t)\dot{B}(\mathbf{r}'0)\right\rangle = 0 \tag{2.13}$$

Let

$$\begin{aligned} W(\beta) = &\quad \langle [A(\mathbf{r}t), B(\mathbf{r}'0)]\rangle \\ = &\quad \langle A(\mathbf{r}t)B(\mathbf{r}'0)\rangle - \langle B(\mathbf{r}'0)A(\mathbf{r}t)\rangle \\ = &\quad \langle A(\mathbf{r}t)B(\mathbf{r}'0)\rangle - \langle A(\mathbf{r}t)B(\mathbf{r}', i\hbar\beta)\rangle \end{aligned} \tag{2.14}$$

$W(\beta = 0) = 0$, so

$$\begin{aligned} W(\beta) = &\quad \int_0^{\beta} -\left\langle A(\mathbf{r}t)\frac{dB(\mathbf{r}', i\hbar\beta')}{d\beta'}\right\rangle d\beta' \\ = &\quad \int_0^{\beta} -i\hbar\left\langle A(\mathbf{r}t)\frac{dB(\mathbf{r}', i\hbar\beta')}{d(i\hbar\beta')}\right\rangle d\beta' \\ = &\quad \int_0^{\beta} i\hbar\left\langle \dot{A}(\mathbf{r}t)B(\mathbf{r}', i\hbar\beta')\right\rangle \end{aligned} \tag{2.15}$$

proved.

- **Classical limit and correlation functions**

By going from QM to classical mechanics, all we have to do is to replace $[\quad,\quad]/i\hbar$ by $[\quad,\quad]_p$, the Poisson bracket, and C_{AB} in Eqn(2.7) by the classical correlation function $\langle A(\mathbf{r}t)B(\mathbf{r}'t')\rangle_{cl}$, where classical dynamical variables A, B can now exchange position. It isn't apparent though why this is true, and when we can do this. Let's rethink the problem in a somehow stupid but rigorous manner: suppose in a lab Li Ju wants to measure the "correlation function" $\langle A(t)B\rangle_m$, where m stands for measurement. The initial states, before any measurement, are energy eigenstates $|\varepsilon\rangle$ with probability $e^{-\beta\varepsilon}/\sum_\varepsilon e^{-\beta\varepsilon}$. From the basic assumptions of quantum mechanics, a measurement of operator B yields one of its eigenvalues b with probability $|\langle b|\varepsilon\rangle|^2$, and the state is immediately *projected* into $|b\rangle$ which continues on. After time evolution $e^{-i\mathcal{H}_0 t/\hbar}$, a measurement on A is made. Suppose

$$\mathcal{H}_0|\varepsilon\rangle = \varepsilon|\varepsilon\rangle \qquad A|a\rangle = a|a\rangle \qquad B|b\rangle = b|b\rangle \tag{2.16}$$

By the process, our "measurement" correlation function is

$$\begin{aligned} \langle A(t)B\rangle_m = & \sum_{\varepsilon ab} e^{-\beta\varepsilon} \cdot b|\langle b|\varepsilon\rangle|^2 \cdot a|\Big\langle a|e^{-i\mathcal{H}_0 t/\hbar}|b\Big\rangle|^2/Z \\ = & \sum_{\varepsilon ab} \langle b|e^{-\beta\mathcal{H}_0}|\varepsilon\rangle\langle\varepsilon|b\rangle b \cdot \Big\langle b|e^{i\mathcal{H}_0 t/\hbar}|a\Big\rangle\Big\langle a|e^{-i\mathcal{H}_0 t/\hbar}|b\Big\rangle a/Z \\ = & \sum_{b} \langle b|e^{-\beta\mathcal{H}_0}|b\rangle\Big\langle b|Be^{i\mathcal{H}_0 t/\hbar}Ae^{-i\mathcal{H}_0 t/\hbar}|b\Big\rangle/Z \end{aligned} \tag{2.17}$$

Obviously $\langle A(t)B\rangle_m$ is a different quantity from the usual $\langle A(t)B\rangle_{QM} = \mathrm{Tr}\rho A(t)B$, and it has to be time-ordered, i.e., we have to tell explicitly which measurement is made first. In the high temperature limit where $\langle b|e^{-\beta\mathcal{H}_0}|b\rangle$ doesn't vary appreciably for those $|b\rangle$'s that contribute to $\langle b|BA(t)|b\rangle$, we can take the factor to be 1

$$\begin{aligned} \langle A(t)B\rangle_m \approx & \sum_b \Big\langle b|Be^{i\mathcal{H}_0 t/\hbar}Ae^{-i\mathcal{H}_0 t/\hbar}|b\Big\rangle/Z \\ = & \ \mathrm{Tr}BA(t)/Z = \mathrm{Tr}A(t)B/Z \end{aligned} \tag{2.18}$$

Thus $\langle A(t)B\rangle_m$ can be approximated by $\langle\{A(t),B\}/2\rangle_{QM}$. In the other limit where $T \to 0$ the "measurement" correlation function would yield $\langle\varepsilon_0|b\rangle\langle b|BA(t)|b\rangle\langle b|\varepsilon_0\rangle$ where $|\varepsilon_0\rangle$ is the ground state wavefunction, again different from the straightforward $\langle\varepsilon_0|A(t)B|\varepsilon_0\rangle$.

This discussion might be useless in practice though, because most experiments are not carried out like this. Take what we called density-density "correlation" function — the available experimental data is the double differential cross-section $d^2\sigma/d\Omega d\omega$, which can be shown rigorously to be proportional to the Fourier transform of $\langle n(\mathbf{r}t)n(\mathbf{r}'t')\rangle_{QM}$, where $n(\mathbf{r}t), n(\mathbf{r}'t')$ are QM particle density operators. We do not actually measure the density at $(\mathbf{r}'t')$, wait till $(\mathbf{r}t)$, and correlate measured eigenvalues (if that's the case the result will be different). Nevertheless as shown by Eqn(2.12) or Eqn(2.9), at small β $\langle[A(\mathbf{r}t), B(\mathbf{r}'t')]\rangle \to 0$, so it doesn't make any difference between $\langle A(\mathbf{r}t)B(\mathbf{r}'t')\rangle_{QM}$ and $\langle B(\mathbf{r}'t')A(\mathbf{r}t)\rangle_{QM}$ at high temperatures. Since in classical mechanics correlation functions are always commutable, and that's the limit QM is going to take, we might as well keep the symmetry all along in making the identification Eqn(2.7).

Thus, in the classical limit $\beta \to 0$, the dynamical susceptibility is, from Eqn(1.16)

$$\langle [A(\mathbf{r}t), B(\mathbf{r}'t')]_p \rangle_{cl} = -2i\chi''_{AB}(\mathbf{rr}', t-t') \tag{2.19}$$

with

$$\chi_{AB}(\mathbf{rr}', \omega) = \chi'_{AB}(\mathbf{rr}', \omega) + i\chi''_{AB}(\mathbf{rr}', \omega) \tag{2.20}$$

and all the symmetry properties and Kramers-Kronig relations still hold. The fluctuation-dissipation theorem in Eqn(2.9) become

$$C_{AB}(\mathbf{rr}', \omega) = \frac{2}{\beta\omega}\chi''_{AB}(\mathbf{rr}', \omega) \tag{2.21}$$

by taking the small β limit. So there is

$$\chi''_{AB}(\mathbf{rr}', \omega) = \frac{i\beta(-i\omega)}{2} C_{AB}(\mathbf{rr}', \omega) \tag{2.22}$$

$$\chi''_{AB}(\mathbf{rr}', t-t') = \frac{i\beta}{2}\dot{C}_{AB}(\mathbf{rr}', t-t') = \frac{i\beta}{2}\left\langle \dot{A}(\mathbf{r}t)B(\mathbf{r}'t')\right\rangle \tag{2.23}$$

This result, without going through Eqn(2.9) and take the $\beta \to 0$ limit, can be directly derived from Eqn(2.19) using classical mechanics

$$\begin{aligned}
\langle [A(t), B]_p \rangle_{cl} &= \int d\Gamma \exp\left(-\beta\mathcal{H}_0(\Gamma)\right) [A(t), B]_p / Z \\
&= -\int d\Gamma [A(t), \exp\left(-\beta\mathcal{H}_0(\Gamma)\right)]_p B / Z \\
&= \beta \int d\Gamma \exp\left(-\beta\mathcal{H}_0(\Gamma)\right) [A(t), \mathcal{H}_0]_p B / Z \\
&= \beta \left\langle \dot{A}(t) B \right\rangle
\end{aligned} \tag{2.24}$$

Most of the time Eqn(2.23) is the form we prefer to use. It is also interesting to compare it with the exact QM expression of Eqn(2.12).

- **Properties of correlation function C_{AB}**

1. As shown in Eqn(2.13), for $\mathcal{H}_0$ with no explicit time dependence

$$\left\langle \dot{A}(t)B\right\rangle + \left\langle A(t)\dot{B}\right\rangle = 0$$

and this still holds true for correlation functions

$$\frac{1}{2}\Big\langle\Big\{\dot{A}(\mathbf{r}t), B(\mathbf{r}')\Big\}\Big\rangle + \frac{1}{2}\Big\langle\Big\{A(\mathbf{r}t), \dot{B}(\mathbf{r}')\Big\}\Big\rangle = 0 \tag{2.25}$$

2. The operation $\langle\{A, B\}\rangle/2$ can be thought of as an inner product (A, B), since it's linear and $(A, A) \geq 0$. By Schwartz's inequality

$$\begin{aligned} |C_{AB}(\mathbf{r}\mathbf{r}', t-t')| = & \frac{1}{2}\,|\langle\{A(\mathbf{r}t), B(\mathbf{r}')\}\rangle| \\ \leq & \frac{1}{2}\sqrt{\langle\{A(\mathbf{r}t), A(\mathbf{r}t)\}\rangle\langle\{B(\mathbf{r}'), B(\mathbf{r}')\}\rangle} \\ = & \sqrt{\langle A^2(\mathbf{r})\rangle\langle B^2(\mathbf{r}')\rangle} \end{aligned} \tag{2.26}$$

Furthermore, from Eqn(2.10), we have

$$\int d\mathbf{r}d\mathbf{r}' f(\mathbf{r}) f^*(\mathbf{r}') C_{AA}(\mathbf{r}\mathbf{r}', \omega) \geq 0 \tag{2.27}$$

so $C_{AA}(\mathbf{r}\mathbf{r}', \omega)$ can be thought of as a *positive definite* matrix if $\mathbf{r}\mathbf{r}'$ are considered to be matrix indices. If the system is spatially translational invariant

$$C_{AA}(\mathbf{r}\mathbf{r}', \omega) = C_{AA}(\mathbf{r} - \mathbf{r}', \omega) \tag{2.28}$$

and by taking $f(\mathbf{r})$ to be $e^{-i\mathbf{k}\cdot\mathbf{r}}$, we have

$$C_{AA}(\mathbf{k}\omega) \geq 0 \tag{2.29}$$

and we can further show that

$$C_{AA}(\mathbf{k}t) \leq C_{AA}(\mathbf{k}, t=0) \tag{2.30}$$

by using Lehmann representation and define inner product in $\mathbf{k}$ subspace, just like in Eqn(2.26).

3. Since

$$C_{AB}(\mathbf{r}\mathbf{r}', \omega) = \hbar\coth\frac{\beta\hbar\omega}{2}\chi''_{AB}(\mathbf{r}\mathbf{r}', \omega)$$

the symmetry properties of C_{AB} are divided into two groups

(a) $\varepsilon_A = \varepsilon_B$: $C_{AB}(\mathbf{rr'}, \omega)$ is real and even in ω

$C_{AB}(\mathbf{rr'}, t)$ is real and even in t

(b) $\varepsilon_A = -\varepsilon_B$: $C_{AB}(\mathbf{rr'}, \omega)$ is imaginary and odd in ω

$C_{AB}(\mathbf{rr'}, t)$ is real and odd in t

Especially, autocorrelation function C_{AA} must be real and even in both t and ω.

Chapter 3

Hydrodynamic Equations and Spin Diffusion

In principle, the knowledge of correlation functions would enable us to determine every property of the system under small perturbation, including the small $\mathbf{k}\omega$, i.e., the hydrodynamic behaviour. In practice however, this is the most difficult part if going *from first principle*, because hydrodynamic regime is characterized by local thermodynamic equilibrium, which is achieved through large numbers of collisions over a long period of time. Thus the straightforward method of perturbation expansion in terms of interaction strength usually breaks down here.

We can study the inverse problem , i.e., how does the phenomenological but acknowledged correct hydrodynamic equations impose constraint on the form of correlation functions in the small $\mathbf{k}\omega$ region. We shall see that they display complicated singular behaviour as $\mathbf{k}, \omega \to 0$ which, if we take the limit in correct order, would yield two kinds of quantities of essential interest: one are the *thermodynamic derivatives* such as static magnetic susceptibility χ, heat capacity C_p, isothermal compressibility κ_T etc. The other kind are transport coefficients such as diffusion constant D, viscosity η, ζ, or thermal conductivity κ. These quantities served as empirical parameters in hydrodynamic equations and must be provided as input.

The story does not end here: with the advance of modern computers people can afford to simulate many-body atomic or molecular systems using Molecular Dynamics (MD) techniques in a fairly large supercell. Correlation functions, as an equilibrium bulk property, can be numerically calculated in these simulations to reasonable accuracy. One important end-product would be these thermodynamic derivatives and transport coefficients. Thus this theoretical hysteric of going “from correlation functions to hydrodynamic behaviour”, or the other way around, is indeed of practical importance. The author has carried out one of these simulations to get the thermal conductivity of irradiated SiC using classical potential.

Let’s consider the simplest example of spin diffusion, which is pretty well realized in liquid He^3: suppose we have a fluid of spin 1/2 particles interacting via velocity- and spin-independent forces, then

$$\mathcal{H}_0 = \sum_i \frac{\mathbf{p}_i^2}{2m} + V(\mathbf{r}_1, ..., \mathbf{r}_N) \tag{3.1}$$

We only consider magnetization in the z-direction

$$M(\mathbf{r}t) = \sum_i \gamma S_{iz}(t) \delta\left(\mathbf{r} - \mathbf{r}_i(t)\right) \tag{3.2}$$

$\mathbf{S}_i(t)$ is the spin angular momentum operator, γ is its ratio to magnetic moment. Since $\sum_i S_{iz}(t)$ commutes with $\mathcal{H}_0$

$$\frac{d}{dt} \int d\mathbf{r} M(\mathbf{r}t) = 0 \tag{3.3}$$

This conservation also has a differential form. Following the derivations in Eqn(1.12), we have

$$\frac{d}{dt} M(\mathbf{r}t) + \nabla \cdot \mathbf{J}^M(\mathbf{r}t) = 0 \tag{3.4}$$

where

$$\mathbf{J}^M(\mathbf{r}t) = \sum_i \gamma S_{iz}(t) \left\{\mathbf{p}_i(t)/2m, \delta\left(\mathbf{r} - \mathbf{r}_i(t)\right)\right\} \tag{3.5}$$

The absorptive part of magnetization-magnetization dynamic susceptibility is just

$$\chi''_{MM}(\mathbf{r}\mathbf{r}', t - t') = \frac{1}{2\hbar} \langle [M(\mathbf{r}t), M(\mathbf{r}'t')] \rangle \tag{3.6}$$

- **Longitudinal f-sum rule**

There is an exact result on $\chi''_{MM}(\mathbf{r}\mathbf{r}', \omega)$ using equal time commutator following the derivations in Eqn(1.33). Since

$$\frac{d}{dt} M(\mathbf{r}t) = -\nabla \cdot \mathbf{J}^M(\mathbf{r}t)$$

and

$$\begin{aligned}\left\langle[\mathbf{J}^M(\mathbf{r}),M(\mathbf{r}')]\right\rangle &= \left\langle\sum_i \frac{\gamma^2 S_{iz}^2}{2m}[\{\mathbf{p}_i,\delta(\mathbf{r}-\mathbf{r}_i)\},\delta(\mathbf{r}'-\mathbf{r}_i)]\right\rangle \\ &= \left\langle\sum_i \frac{\gamma^2 S_{iz}^2}{2m}\{\delta(\mathbf{r}-\mathbf{r}_i),[\mathbf{p}_i,\delta(\mathbf{r}'-\mathbf{r}_i)]\}\right\rangle \\ &= \left\langle\sum_i \frac{\gamma^2 S_{iz}^2}{m} i\hbar\delta(\mathbf{r}-\mathbf{r}_i)\nabla'\delta(\mathbf{r}'-\mathbf{r})\right\rangle \\ &= \frac{\gamma^2}{m}\frac{1}{3}(\frac{1}{2})(\frac{3}{2})\hbar^2\cdot i\hbar\langle n(\mathbf{r})\rangle\nabla'\delta(\mathbf{r}'-\mathbf{r}) \\ &= \frac{i\gamma^2\hbar^3\langle n(\mathbf{r})\rangle}{4m}\nabla'\delta(\mathbf{r}'-\mathbf{r}) \qquad (3.7)\end{aligned}$$

So from Eqn(1.33), we have

$$\begin{aligned}\int\frac{d\omega}{\pi}\omega\chi''_{MM}(\mathbf{r}\mathbf{r}',\omega) &= -\frac{i}{\hbar}\nabla\cdot\left\langle[\mathbf{J}^M(\mathbf{r}),M(\mathbf{r}')]\right\rangle \\ &= -\frac{\gamma^2\hbar^2\langle n(\mathbf{r})\rangle}{4m}\nabla^2\delta(\mathbf{r}'-\mathbf{r}) \qquad (3.8)\end{aligned}$$

When the system is translational invariant, $\chi''_{MM}(\mathbf{r}\mathbf{r}',\omega)=\chi''_{MM}(\mathbf{r}-\mathbf{r}',\omega)$ and so $\langle n(\mathbf{r})\rangle = n$. There is

$$\int\frac{d\omega}{\pi}\omega\chi''_{MM}(\mathbf{k}\omega)=\frac{\gamma^2\hbar^2 nk^2}{4m} \qquad (3.9)$$

This result is widely referred in literature as the longitudinal f-sum rule.

When the system varies slowly in space and time, we usually acknowledge the following hydrodynamic equation

$$\left\langle\mathbf{J}^M(\mathbf{r}t)\right\rangle = -D\nabla\langle M(\mathbf{r}t)\rangle \qquad (3.10)$$

where D is the *spin diffusion coefficient*, a transport coefficient to be determined. Combining this with Eqn(3.4), we arrive at

$$\frac{\partial}{\partial t}\langle M(\mathbf{r}t)\rangle = D\nabla^2\langle M(\mathbf{r}t)\rangle \qquad (3.11)$$

The method of linking hydrodynamic equations with our previous linear response formalism is to *devise* an "idea experiment" which could lead to results from the two different ways, and then equate them. In this case, we imagine preparing the system at $t\leq 0$ by adding the following magnetic field in the z-direction

$$H(\mathbf{r}t) = \begin{cases} H(\mathbf{r})e^{\varepsilon t} & t \leq 0 \\ \\ 0 & t > 0 \end{cases} \tag{3.12}$$

where ε is infinitesimal positive number. The perturbation to the Hamiltonian is of course

$$\mathcal{H}_I(t') = -\int d\mathbf{r}' M(\mathbf{r}'t')H(\mathbf{r}'t') \tag{3.13}$$

• **Hydrodynamic approach:**

At $t = 0$ $H(\mathbf{r}t) = H(\mathbf{r})$, and it had almost been so for quite a long time (ε is very small). For an observer in the laboratory, he would write down

$$M(\mathbf{r}, t = 0) = \chi H(\mathbf{r}) \tag{3.14}$$

where χ is the *static magnetic susceptibility*, an empirical parameter to be determined. χ is also a thermodynamic derivative

$$\chi = \left.\frac{\partial M}{\partial H}\right)_{H=0} \tag{3.15}$$

Taking the Fourier transform we would have

$$M(\mathbf{k}, t = 0) = \chi H(\mathbf{k}) \tag{3.16}$$

After $t = 0$ there is no external magnetic field and all finite wave-vector magnetizations will relax to zero, i.e., spatial inhomogeneity will be erased due to spin diffusion. The system should be able to be described by Eqn(3.11) if $H(\mathbf{r})$ is of long length-scale. From now on we'll omit the bracket around measurables if without special notice. Taking complex Laplace transform on both sides

$$-iz\tilde{M}(\mathbf{k}z) - M(\mathbf{k}, t = 0) = -Dk^2\tilde{M}(\mathbf{k}z) \tag{3.17}$$

then it predicts

$$\tilde{M}(\mathbf{k}z) = \frac{M(\mathbf{k}, t = 0)}{-iz + Dk^2} = \frac{\chi H(\mathbf{k})}{-iz + Dk^2} \tag{3.18}$$

The pole at $-iDk^2$ is characteristic of all pure diffusive processes.

- **Linear response approach:**

An equilibrium system with no external magnetic field should have no magnetization. If we use Eqn(1.18), Eqn(3.13), we shall have

$$M(\mathbf{r}t) = \begin{cases} \int_{-\infty}^{t} 2i\chi''_{MM}(\mathbf{r}\mathbf{r}', t-t')H(\mathbf{r}')e^{\varepsilon t'}d\mathbf{r}'dt' & t \leq 0 \\ \\ \int_{-\infty}^{0} 2i\chi''_{MM}(\mathbf{r}\mathbf{r}', t-t')H(\mathbf{r}')e^{\varepsilon t'}d\mathbf{r}'dt' & t > 0 \end{cases} \tag{3.19}$$

For $t > 0$

$$\begin{aligned} M(\mathbf{r}t) = & \int_{-\infty}^{0} 2i\chi''_{MM}(\mathbf{r}\mathbf{r}', t-t')H(\mathbf{r}')e^{\varepsilon t'}d\mathbf{r}'dt' \\ = & \int_{-\infty}^{0} 2i\int \frac{d\omega}{2\pi}\chi''_{MM}(\mathbf{r}\mathbf{r}', \omega)H(\mathbf{r}')e^{-i\omega(t-t')+\varepsilon t'}d\mathbf{r}'dt' \\ = & \int \frac{d\omega}{\pi}\frac{\chi''_{MM}(\mathbf{r}\mathbf{r}', \omega)}{w}e^{-i\omega t}H(\mathbf{r}')d\mathbf{r}' \end{aligned} \tag{3.20}$$

and so

$$M(\mathbf{r}, t=0) = \int \frac{d\omega}{\pi}\frac{\chi''_{MM}(\mathbf{r}\mathbf{r}', \omega)}{w}H(\mathbf{r}')d\mathbf{r}' \tag{3.21}$$

For translational invariant systems $\chi''_{MM}(\mathbf{r}\mathbf{r}', \omega) = \chi''_{MM}(\mathbf{r}-\mathbf{r}', \omega)$ and the above equations are all in spatial convolution form, so

$$\begin{aligned} M(\mathbf{k}, t=0) = & \int \frac{d\omega}{\pi}\frac{\chi''_{MM}(\mathbf{k}\omega)}{w}H(\mathbf{k}) \\ = & \chi_{MM}(\mathbf{k}, z=0)H(\mathbf{k}) \end{aligned} \tag{3.22}$$

the last line come from Eqn(10). And

$$M(\mathbf{k}t) = \int \frac{d\omega}{\pi}\frac{\chi''_{MM}(\mathbf{k}\omega)}{w}e^{-i\omega t}H(\mathbf{k}) \tag{3.23}$$

$$\begin{aligned} \tilde{M}(\mathbf{k}z) = & \int_0^{+\infty} e^{izt}M(\mathbf{k}t)dt \\ = & \int_0^{+\infty} e^{izt}\int \frac{d\omega}{\pi}\frac{\chi''_{MM}(\mathbf{k}\omega)}{w}e^{-i\omega t}H(\mathbf{k})dt \\ = & \int \frac{d\omega}{\pi i}\frac{\chi''_{MM}(\mathbf{k}\omega)}{\omega(\omega-z)}H(\mathbf{k}) \end{aligned} \tag{3.24}$$

By comparing Eqn(3.21) with Eqn(3.14) and Eqn(3.24) with Eqn(3.18) we see that at small $\mathbf{k}, \omega$, there must be

$$\chi = \lim_{k\to 0} \chi''_{MM}(\mathbf{k}, z=0) = \lim_{k\to 0} \int \frac{d\omega}{\pi} \frac{\chi''_{MM}(\mathbf{k}\omega)}{\omega} \tag{3.25}$$

and by taking the $z = w + i\varepsilon$ limit

$$\text{from} \qquad \text{Eqn(3.18)}: \quad \mathrm{Re}\frac{\tilde{M}(\mathbf{k}, \omega + i\varepsilon)}{H(\mathbf{k})} = \mathrm{Re}\frac{\chi}{-iz + Dk^2} = \frac{\chi D k^2}{\omega^2 + (Dk^2)^2} \tag{3.26}$$

$$\text{from} \qquad \text{Eqn(3.24)}: \quad \mathrm{Re}\frac{\tilde{M}(\mathbf{k}, \omega + i\varepsilon)}{H(\mathbf{k})} = \int \frac{d\omega'}{\pi} \frac{\chi''_{MM}(\mathbf{k}\omega')}{\omega'} \mathrm{Im}\frac{1}{\omega' - w - i\varepsilon} = \frac{\chi''_{MM}(\mathbf{k}\omega)}{\omega} \tag{3.27}$$

Thus, at small $\mathbf{k}\omega$, $\chi''_{MM}(\mathbf{k}\omega)$ must be of the form

$$\chi''_{MM}(\mathbf{k}\omega) = \frac{\chi D k^2 \omega}{\omega^2 + (Dk^2)^2} \tag{3.28}$$

and the magnetization-magnetization correlation function C_{MM}, by virtue of the fluctuation-dissipation theorem, is

$$C_{MM}(\mathbf{k}\omega) = \frac{\chi D k^2}{\omega^2 + (Dk^2)^2} \hbar\omega \coth\frac{\beta\hbar\omega}{2} \tag{3.29}$$

- **Observation No.1**

When $\mathbf{k} \to 0$, Eqn(3.28) predicts that $\chi''_{MM}(\mathbf{k}\omega)/\omega$ (and correlation function $C_{MM}(\mathbf{k}\omega)$) has the limiting behaviour of a delta-function $\pi\chi\delta(\omega)$ $(2\pi k_B T \chi \delta(\omega))$. This is a general conclusion for all response/correlation functions of densities of conserved variables. It could be seen from Eqn(3.20) — since the total magnetization

$$\int M(\mathbf{r}t) d\mathbf{r} = \int \frac{d\omega}{\pi} \frac{\chi''_{MM}(\mathbf{k}=0, \omega)}{\omega} e^{-i\omega t} H(\mathbf{r}') d\mathbf{r}' \tag{3.30}$$

is a constant of time after $t = 0$, there can be no non-zero frequency components when

$\mathbf{k} \to 0$.

Eqn(3.29) can be utilized to get the static magnetic susceptibility χ

$$\lim_{k\to 0} C_{MM}(\mathbf{k}\omega) = \pi\chi\delta\left(\omega\right)\hbar\omega\coth\frac{\beta\hbar\omega}{2} = 2\pi k_B T\chi\delta\left(\omega\right) \tag{3.31}$$

there must be

$$\begin{aligned}\chi = \quad & \frac{1}{k_B T}\lim_{k\to 0}\int\frac{d\omega}{2\pi}C_{MM}(\mathbf{k}\omega) \\ = \quad & \frac{1}{k_B T}\lim_{k\to 0}C_{MM}(\mathbf{k}, t=0) \\ = \quad & \frac{1}{k_B T}\lim_{k\to 0}\int\frac{1}{2}\langle\{M(\mathbf{r}), M(\mathbf{0})\}\rangle e^{-i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r} \\ = \quad & \frac{1}{2k_B T}\int\langle\{M(\mathbf{r}), M(\mathbf{0})\}\rangle d\mathbf{r}\end{aligned} \tag{3.32}$$

In this case the last $\mathbf{k} \to 0$ limit should be taken with ease becase in common materials $\langle\{M(\mathbf{r}), M(\mathbf{0})\}\rangle$ decays to zero with absolute convergence, as this is the case for most $\langle\{A(\mathbf{r}) - \langle A\rangle, B(\mathbf{0}) - \langle B\rangle\}\rangle$ functions. However for those systems with long range correlations such as Coloumb systems or superfluids, the $\mathbf{k} \to 0$ limit displays pathological behaviour as the $\mathbf{k} = 0$ value would depend on the exact shape of the boundary. By then the $\mathbf{k} \to 0$ limit actually means picking a k such that $\frac{2\pi}{L} \ll k \ll \frac{2\pi}{A}$, where L is size of the system and A is the length scale of interest (with this constraint, $\mathbf{k} \to 0$ as $L \to +\infty$).

Lastly , Eqn(3.32) could be expressed in terms of total magnetization $M = \int d\mathbf{r}M(\mathbf{r})$ by taking into account the translational invariance of the system. Then

$$\chi = \frac{\langle M^2\rangle}{k_B T\Omega} \tag{3.33}$$

where Ω is the total volume. This is the form of "fluctuation formulas" that we often use to get thermodynamic derivatives, which can also be arrived at by expanding the equilibrium density matrix.

- **Observation No.2**

The spin diffusion coefficient D can be gotten from Eqn(3.28)

$$D\chi = \quad \lim_{\omega\to 0}\lim_{k\to 0}\frac{w}{k^2}\chi''_{MM}(\mathbf{k}\omega)$$

$$
\begin{aligned}
&= \lim_{\omega\to 0}\lim_{k\to 0}\frac{\omega\tanh\beta\hbar\omega/2}{\hbar k^2}C_{MM}(\mathbf{k}\omega) \\
&= \lim_{\omega\to 0}\frac{\tanh\beta\hbar\omega/2}{\hbar\omega}\Big(\lim_{k\to 0}\frac{\omega^2}{k^2}\int dtd\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega t}\langle\{M(\mathbf{r}t),M(\mathbf{0}0)\}\rangle/2\Big) \\
&= \frac{\beta}{4}\lim_{\omega\to 0}\lim_{k\to 0}\frac{\omega^2}{k^2}\int dtd\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega t}\langle\{M(\mathbf{r}t),M(\mathbf{0}0)\}\rangle
\end{aligned}
\tag{3.34}
$$

But

$$
\begin{aligned}
&\int dte^{i\omega t}\omega^2\langle\{M(\mathbf{r}t),M(\mathbf{0}0)\}\rangle \\
=\;& -\int dte^{i\omega t}\Big\langle\Big\{\ddot{M}(\mathbf{r}t),M(\mathbf{0}0)\Big\}\Big\rangle \\
=\;& \int dte^{i\omega t}\Big\langle\Big\{\dot{M}(\mathbf{r}t),\dot{M}(\mathbf{0}0)\Big\}\Big\rangle \\
=\;& \int dte^{i\omega t}\Big\langle\Big\{\nabla\cdot\mathbf{J}^M(\mathbf{r}t),\nabla\cdot\mathbf{J}^M(\mathbf{0}0)\Big\}\Big\rangle
\end{aligned}
\tag{3.35}
$$

So

$$
\begin{aligned}
D\chi =\;& \frac{\beta}{4}\lim_{\omega\to 0}\lim_{k\to 0}\frac{1}{k^2}\int dtd\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega t}\Big\langle\Big\{\mathbf{k}\cdot\mathbf{J}^M(\mathbf{r}t),\mathbf{k}\cdot\mathbf{J}^M(\mathbf{0}0)\Big\}\Big\rangle \\
=\;& \frac{\beta}{4}\lim_{\omega\to 0}\int dtd\mathbf{r}e^{i\omega t}\Big\langle\Big\{\mathbf{J}_x^M(\mathbf{r}t),\mathbf{J}_x^M(\mathbf{0}0)\Big\}\Big\rangle \\
=\;& \frac{\beta}{4}\int dtd\mathbf{r}\Big\langle\Big\{\mathbf{J}_x^M(\mathbf{r}t),\mathbf{J}_x^M(\mathbf{0}0)\Big\}\Big\rangle
\end{aligned}
\tag{3.36}
$$

as we pick an arbitary direction x to be the direction of $\mathbf{k}$ in the isotropic fluid.

Notice that we can only get to final result Eqn(3.36) by taking the correct sequence of limit $\lim_{\omega\to 0}\lim_{k\to 0}$. We would get zero if the other way around, as indicated by the hydrodynamic prediction Eqn(3.28), because then in Eqn(3.35)

$$\lim_{\omega\to 0}\omega^2\int dte^{i\omega t}\langle\{M(\mathbf{r}t),M(\mathbf{0}0)\}\rangle = 0 \tag{3.37}$$

as $\langle\{M(\mathbf{r}t),M(\mathbf{0}0)\}\rangle$ must be a finite and decay-to-zero function of t. The two-sided Fourier transform is properly defined through replacing ω by $\omega+i\varepsilon$ at $t>0$ and $\omega-i\varepsilon$ at $t<0$, thus even for a temporal constant its Fourier transform would give $2\varepsilon/(\omega^2+\varepsilon^2)$. Since

$$\lim_{\omega\to 0}\frac{2\omega^2\varepsilon}{\omega^2+\varepsilon^2} = 0 \tag{3.38}$$

for any ε, the expression is bound to go to zero.

- **Observation No.3**

We see that the hydrodynamic form of $\chi''_{MM}(\mathbf{k}\omega)$ in Eqn(3.28) will always satisfy the exact sum rule

$$\chi(\mathbf{k}) = \int \frac{d\omega}{\pi} \frac{\chi(\mathbf{k})Dk^2}{\omega^2 + (Dk^2)^2} = \int \frac{d\omega}{\pi} \frac{\chi''_{MM}(\mathbf{k}\omega)}{\omega} \tag{3.39}$$

for *all* $\mathbf{k}$ if we revise our empirical law Eqn(3.16) by changing χ to $\chi(\mathbf{k})$, a wave-vector dependent static magnetic susceptibility to include non-local effects. However, another exact result, sum rule Eqn(3.9), is entirely missed by the hydrodynamic expression. The physical reason being that we had assumed $\mathbf{J}^M(\mathbf{r}t)$ to respond *instantly* to any gradient of magnetization density in the system, but actually it requires a short time. We could improve it by making a *relaxation time* approximation, whereas we revise our hydrodynamic law Eqn(3.10) to be

$$(\frac{\partial}{\partial t} + \frac{1}{\tau})\mathbf{J}^M(\mathbf{r}t) = -\frac{D}{\tau}\nabla M(\mathbf{r}t) \tag{3.40}$$

and so

$$(\frac{\partial^2}{\partial t^2} + \frac{1}{\tau}\frac{\partial}{\partial t})M(\mathbf{r}t) = \frac{D}{\tau}\nabla^2 M(\mathbf{r}t) \tag{3.41}$$

By using the initial condition

$$\langle M(\mathbf{r}, t=0)\rangle = \chi H(\mathbf{r}) \qquad \frac{\partial}{\partial t}\langle M(\mathbf{r}t)\rangle\bigg|_{t=0} = 0 \tag{3.42}$$

which must be satisfied by our "idea experiment" Eqn(3.12). Then there is

$$\frac{\tilde{M}(\mathbf{k}z)}{H(\mathbf{k})} = \frac{\chi}{-iz + \frac{Dk^2/\tau}{-iz+1/\tau}} = \int \frac{d\omega}{\pi i} \frac{\chi''_{MM}(\mathbf{k}\omega)}{\omega(\omega - z)} \tag{3.43}$$

such that if we let

$$\tau = \frac{4mD\chi}{n\gamma^2\hbar^2} \tag{3.44}$$

the exact sum rule Eqn(3.9) would be satisfied. Eqn(3.43) is called a *recursion* form, which can be iterated to higher and higher order. To see how it works expand Eqn(3.43) in power series of $1/z^n$.

Chapter 4

Transport in Normal One-Component Fluid

The spin diffusion problem is extremely simple because in hydrodynamic regime, the diffusion of magnetization density is independent of other 1st-order fluctuations, since even in an otherwise perfectly homogeneous fluid it will still happen due to frequent interdiffusion. Fluctuations such as particle density only contribute to the second order. Thus it is plausible to write down Eqn(3.10) with a single empirical constant D. Such is not true if we want to investigate other degrees of freedom because they are all coupled together in linear order. It is not possible, say, to set up a heat current by applying a temperature gradient without perturbing neither of the other two parameters: pressure and density, which will in turn induce particle flow.

Let's define particle density to be $n(\mathbf{r}t)$, momentum density $\mathbf{j}(\mathbf{r}t)$ and energy density $\epsilon(\mathbf{r}t)$. Then

$$\frac{\partial}{\partial t}n(\mathbf{r}t) + \nabla\cdot\mathbf{j}(\mathbf{r}t)/m = 0 \tag{4.1}$$

$$\frac{\partial}{\partial t}\mathbf{j}(\mathbf{r}t) + \nabla\cdot\tau(\mathbf{r}t) = 0 \tag{4.2}$$

$$\frac{\partial}{\partial t}\epsilon(\mathbf{r}t) + \nabla\cdot\mathbf{j}^{\epsilon}(\mathbf{r}t) = 0 \tag{4.3}$$

where $\tau(\mathbf{r}t)$ is the local stress tensor and $\mathbf{j}^{\epsilon}(\mathbf{r}t)$ is the energy flux. Notice that although these are certainly true as hydrodynamic equations, they're still most likely to hold if we take $n(\mathbf{r}t), \mathbf{j}(\mathbf{r}t), \epsilon(\mathbf{r}t)$ to be QM operators, whereas Eqn(4.2),Eqn(4.3) would become the definition of $\tau(\mathbf{r}t), \mathbf{j}^{\epsilon}(\mathbf{r}t)$ in terms of position and momentum operators. Their specific forms would depend on the Hamiltonian. The definition of $\epsilon(\mathbf{r}t)$ might be bit ambigious when the interactions are not pairwise, but it doesn't influence anything in the long wavelength.

We thus set out to make several 1st-order approximations. We take our reference system to be rest and uniform fluid, then the average density n, averge energy density ϵ, average pressure p and the average temperature T would be zeroth order quantities. Their variations at $(\mathbf{r}t)$ would be the 1st order, in addition with the fluxes $\mathbf{j}(\mathbf{r}t)$,$\mathbf{j}^{\epsilon}(\mathbf{r}t)$, the off-diagonal components of $\tau(\mathbf{r}t)$ and velocity field $\mathbf{v}(\mathbf{r}t)$. If we write one 1st order quantity in terms of other 1st order quantities, then only zeroth order coefficients are needed. So

$$\mathbf{j}(\mathbf{r}t) = mn\mathbf{v}(\mathbf{r}t) \tag{4.4}$$

The hydrodynamic form of the stress tensor is given by

$$\tau_{ij}(\mathbf{r}t) = \delta_{ij}p(\mathbf{r}t) - \eta(\frac{\partial v_i(\mathbf{r}t)}{\partial r_j} + \frac{\partial v_j(\mathbf{r}t)}{\partial r_i}) - \delta_{ij}(\zeta - \frac{2}{3}\eta)\nabla\cdot\mathbf{v}(\mathbf{r}t) \tag{4.5}$$

where η is called the *viscosity* or *shear viscosity* and ζ the *bulk viscosity.* This form should work fine for fluids because they are characterized by the loss of shear modulus. And isotropy would require it to be of this form in terms of $\mathbf{v}(\mathbf{r}t)$ with only two coupling constants.

It took some thought to justify the hydrodynamic form of the energy current $\mathbf{j}^{\epsilon}(\mathbf{r}t)$. First we realize that *heat conduction* is solely dependent on temperature differences: two objects would not exchange heat if they are isothermal, although they might be different in pressure or density (thermodynamically it's equivalent to saying that S and T are conjugate variables). So let's only consider the adiabatic situation first: imagine that we trace a fixed number of atoms which form a cell and occupy volume V. The cell floats in the fluid, and after some time it has changed from V to $V + \triangle V$. Since it's adiabatic

$$\begin{aligned} 0 = \quad & \triangle E + p\triangle V = \triangle(\epsilon V) + p\triangle V \\ = \quad & (\epsilon + p)\triangle V + V\triangle\epsilon \end{aligned} \tag{4.6}$$

If we move our origin with the cell, we see that $\triangle V$ is caused by the flux of atoms out of the original cell boundary $\mathcal{S}$ and setting on a new boundary $\mathcal{S}'$. $\triangle V$ is just the surface integral

$$\triangle V = \int_{\mathcal{S}} \mathbf{v}(\mathbf{r}t)\triangle t \cdot \mathbf{n} dS \tag{4.7}$$

where $\mathbf{v}(\mathbf{r}t)$ is the relative velocity with respect to the moving origin. We notice that the energy density change inside $\mathcal{S}$ in Eqn(4.6) is linked with this particle flux out of $\mathcal{S}$. We then have

$$\triangle \epsilon = -\frac{\epsilon + p}{V}\triangle V = -\frac{\Delta t}{V}\int (\epsilon + p)\mathbf{v}(\mathbf{r}t) \cdot \mathbf{n} dS \tag{4.8}$$

so $(\epsilon + p)\mathbf{v}(\mathbf{r}t)$ must be the energy current. Due to Galilean invariance this must be true for the entire system. So

$$\mathbf{j}^{\epsilon}(\mathbf{r}t) = (\epsilon + p)\mathbf{v}(\mathbf{r}t) \tag{4.9}$$

Then we add in the heat flux

$$\mathbf{j}^{\epsilon}(\mathbf{r}t) = (\epsilon + p)\mathbf{v}(\mathbf{r}t) - \kappa \nabla T(\mathbf{r}t) \tag{4.10}$$

where κ is the thermal conductivity, another empirical parameter to be determined.

With Eqn(4.5) we have

$$\begin{aligned}\nabla \cdot \tau = & \quad \nabla p - \eta \nabla(\nabla \cdot \mathbf{v}(\mathbf{r}t)) - \eta \nabla^2 \mathbf{v}(\mathbf{r}t) - (\zeta - \frac{2}{3}\eta)\nabla(\nabla \cdot \mathbf{v}(\mathbf{r}t)) \\ = & \quad \nabla p - \eta \nabla^2 \mathbf{v}(\mathbf{r}t) - (\zeta + \frac{1}{3}\eta)\nabla(\nabla \cdot \mathbf{v}(\mathbf{r}t))\end{aligned} \tag{4.11}$$

plug into Eqn(4.2)

$$\frac{\partial}{\partial t}\mathbf{j}(\mathbf{r}t) + \nabla p(\mathbf{r}t) - \frac{\eta}{mn}\nabla^2 \mathbf{j}(\mathbf{r}t) - \frac{\zeta + \eta/3}{mn}\nabla(\nabla \cdot \mathbf{j}(\mathbf{r}t)) = 0 \tag{4.12}$$

At this time we seperate $\mathbf{j}(\mathbf{r}t)$ into longitudinal and transverse parts

$$\begin{cases} \mathbf{j}(\mathbf{r}t) = \mathbf{j}_l(\mathbf{r}t) + \mathbf{j}_t(\mathbf{r}t) \\ \nabla \cdot \mathbf{j}_t(\mathbf{r}t) = \nabla \times \mathbf{j}_l(\mathbf{r}t) = 0 \end{cases} \tag{4.13}$$

If we Fourier transform $\mathbf{j}(\mathbf{r}t)$, we see that $\mathbf{j}_l(\mathbf{k}t)$ is in the direction of $\mathbf{k}$ while $\mathbf{j}_t(\mathbf{k}t)$ is perpendicular. So if we Fourier transform Eqn(4.12), the transverse current would be automatically seperated out:

$$\frac{\partial}{\partial t}\mathbf{j}_t(\mathbf{k}t) + \frac{\eta k^2}{mn}\mathbf{j}_t(\mathbf{k}t) = 0 \tag{4.14}$$

which by doing the complex Laplace transform, we would have

$$\tilde{\mathbf{j}_t}(\mathbf{k}z) = \frac{mn\mathbf{v}_t(\mathbf{k}, t=0)}{-iz + ak^2} \tag{4.15}$$

where $a = \eta/mn$ is the *transverse diffusion coefficient.* We can see from here that the transverse momentum current is a pure diffusion process, and is entirely decoupled from other degrees of freedom.

We can also take Eqn(4.1) into Eqn(4.12), then

$$-m\frac{\partial^2}{\partial t^2}n(\mathbf{r}t) + \nabla^2 p(\mathbf{r}t) - \frac{\zeta + 4\eta/3}{mn}\nabla^2(-m\frac{\partial}{\partial t}n(\mathbf{r}t)) = 0 \tag{4.16}$$

So

$$\left[-m\frac{\partial^2}{\partial t^2} + \frac{\zeta + 4\eta/3}{n}\frac{\partial}{\partial t}\nabla^2\right] n(\mathbf{r}t) + \nabla^2 p(\mathbf{r}t) = 0 \tag{4.17}$$

By taking Eqn(4.10) into Eqn(4.3), we also get

$$\begin{aligned}&\frac{\partial}{\partial t}\epsilon(\mathbf{r}t) + (\epsilon + p)\nabla\cdot\mathbf{v}(\mathbf{r}t) - \kappa\nabla^2 T(\mathbf{r}t) = 0\\ &\frac{\partial}{\partial t}[\epsilon(\mathbf{r}t) - \frac{\epsilon + p}{n}n(\mathbf{r}t)] - \kappa\nabla^2 T(\mathbf{r}t) = 0\end{aligned} \tag{4.18}$$

Let's define

$$q(\mathbf{r}t) = \epsilon(\mathbf{r}t) - \frac{\epsilon + p}{n}n(\mathbf{r}t) \tag{4.19}$$

$q(\mathbf{r}t)$ could be identified as the *density of heat energy* because

$$TdS = (\epsilon + p)dV + Vd\epsilon \qquad \frac{T}{V}dS = d\epsilon + \frac{\epsilon + p}{V}dV = d\epsilon - \frac{e + p}{n}dn \tag{4.20}$$

(the number of particles we're studying is chosen to be fixed) Then

$$\frac{\partial}{\partial t}q(\mathbf{r}t) - \kappa\nabla^2 T(\mathbf{r}t) = 0 \tag{4.21}$$

With this equation and Eqn(4.17), we see that the problem has two sets of independent variables $\{n(\mathbf{r}t), q(\mathbf{r}t)\}$ and $\{p(\mathbf{r}t), T(\mathbf{r}t)\}$. They are linked by thermodynamic relations because we assume local thermodynamic equilibrium

$$\left\{\begin{array}{l} T(\mathbf{r}t) = \left.\frac{\partial T}{\partial n}\right)_S n(\mathbf{r}t) + \left.\frac{\partial T}{\partial S}\right)_n \frac{V}{T} q(\mathbf{r}t) \\ \\ p(\mathbf{r}t) = \left.\frac{\partial p}{\partial n}\right)_S n(\mathbf{r}t) + \left.\frac{\partial P}{\partial S}\right)_n \frac{V}{T} q(\mathbf{r}t) \end{array}\right. \tag{4.22}$$

$$\left\{\begin{array}{l} n(\mathbf{r}t) = \left.\frac{\partial n}{\partial p}\right)_T p(\mathbf{r}t) + \left.\frac{\partial n}{\partial T}\right)_p T(\mathbf{r}t) \\ \\ q(\mathbf{r}t) = \frac{T}{V} \left.\frac{\partial S}{\partial p}\right)_T p(\mathbf{r}t) + \frac{T}{V} \left.\frac{\partial S}{\partial T}\right)_p T(\mathbf{r}t) \end{array}\right. \tag{4.23}$$

where by $T(\mathbf{r}t)$ we really mean $\delta T(\mathbf{r}t)$ etc. Write the above equations in matrix form and the following identity must hold

$$\begin{aligned} & \begin{bmatrix} \left.\frac{\partial T}{\partial n}\right)_S & \left.\frac{\partial T}{\partial S}\right)_n \frac{V}{T} \\ \\ \left.\frac{\partial p}{\partial n}\right)_S & \left.\frac{\partial P}{\partial S}\right)_n \frac{V}{T} \end{bmatrix} \begin{bmatrix} \left.\frac{\partial n}{\partial p}\right)_T & \left.\frac{\partial n}{\partial T}\right)_p \\ \\ \frac{T}{V} \left.\frac{\partial S}{\partial p}\right)_T & \frac{T}{V} \left.\frac{\partial S}{\partial T}\right)_p \end{bmatrix} \\ = & \begin{bmatrix} \left.\frac{\partial T}{\partial n}\right)_S \left.\frac{\partial n}{\partial p}\right)_T + \left.\frac{\partial T}{\partial S}\right)_n \left.\frac{\partial S}{\partial p}\right)_T & \left.\frac{\partial T}{\partial n}\right)_S \left.\frac{\partial n}{\partial T}\right)_p + \left.\frac{\partial T}{\partial S}\right)_n \left.\frac{\partial S}{\partial T}\right)_p \\ \\ \left.\frac{\partial P}{\partial n}\right)_S \left.\frac{\partial n}{\partial p}\right)_T + \left.\frac{\partial P}{\partial S}\right)_n \left.\frac{\partial S}{\partial p}\right)_T & \left.\frac{\partial p}{\partial n}\right)_S \left.\frac{\partial n}{\partial T}\right)_p + \left.\frac{\partial p}{\partial S}\right)_n \left.\frac{\partial S}{\partial T}\right)_p \end{bmatrix} \\ = & \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \end{aligned} \tag{4.24}$$

We define

$$mc_S^2 = \left.\frac{\partial p}{\partial n}\right)_S \qquad mnc_p = \frac{T}{V} \left.\frac{\partial S}{\partial T}\right)_p \qquad mnc_V = \frac{T}{V} \left.\frac{\partial S}{\partial T}\right)_V \tag{4.25}$$

where c_S is the *adiabatic speed of sound*, and remember that

$$C_p - C_V = -T \left.\frac{\partial S}{\partial V}\right)_T \left.\frac{\partial S}{\partial p}\right)_T \qquad \left.\frac{\partial S}{\partial p}\right)_T = - \left.\frac{\partial V}{\partial T}\right)_p = \frac{V}{n} \left.\frac{\partial n}{\partial T}\right)_p \tag{4.26}$$

$$\gamma = \frac{c_p}{c_v} = 1 - \left.\frac{\partial P}{\partial S}\right)_V \left.\frac{\partial S}{\partial p}\right)_T = 1 - \left.\frac{\partial T}{\partial n}\right)_S \left.\frac{\partial n}{\partial T}\right)_p \tag{4.27}$$

We can show from the matrix identity that

$$\left\{\begin{array}{l} \left.\frac{\partial T}{\partial n}\right)_S \left.\frac{\partial n}{\partial p}\right)_T + \frac{T}{mn^2c_V} \left.\frac{\partial n}{\partial T}\right)_p = 0 \\ \left.\frac{\partial T}{\partial n}\right)_S \left.\frac{\partial n}{\partial T}\right)_p = 1 - \gamma \\ mc_S^2 \left.\frac{\partial n}{\partial p}\right)_T = \gamma \\ c_S^2 \left.\frac{\partial n}{\partial T}\right)_p + \frac{n^2c_p}{T} \left.\frac{\partial T}{\partial n}\right)_S = 0 \end{array}\right. \tag{4.28}$$

Remember that everything was taken with respect to constant number of particles, so $\partial \ln V = -\partial \ln n$.

If we define

$$b = \frac{\zeta + 4\eta/3}{mn} \tag{4.29}$$

to be the *longitudinal diffusion coefficient*, and Fourier transform Eqn(4.17),Eqn(4.21) to $\mathbf{k}$ space

$$\left\{\begin{array}{l} m(\frac{\partial^2}{\partial t^2} + bk^2\frac{\partial}{\partial t})n(\mathbf{k}t) + k^2 p(\mathbf{k}t) = 0 \\ \\ \frac{\partial}{\partial t}q(\mathbf{k}t) + \kappa k^2 T(\mathbf{k}t) = 0 \end{array}\right. \tag{4.30}$$

From now on we'll use $\{n(\mathbf{k}t), q(\mathbf{k}t)\}$ as dynamical variables. So take in Eqn(4.22)

$$\left\{\begin{array}{l} \left(m\frac{\partial^2}{\partial t^2} + mbk^2\frac{\partial}{\partial t} + \left.\frac{\partial p}{\partial n}\right)_S k^2\right)n(\mathbf{k}t) + \frac{V}{T}\left.\frac{\partial p}{\partial S}\right)_n k^2 q(\mathbf{k}t) = 0 \\ \\ \left(\frac{\partial}{\partial t} + \frac{\kappa V}{T}\left.\frac{\partial T}{\partial S}\right)_n k^2\right)q(\mathbf{k}t) + \kappa \left.\frac{\partial T}{\partial n}\right)_S k^2 n(\mathbf{k}t) = 0 \end{array}\right. \tag{4.31}$$

Let's further assume that at $t = 0$, the longitudinal momentum current $\mathbf{j}_l(\mathbf{k}t)$ are all zero, so that the first-order time derivative of $n(\mathbf{k}t)$ is zero. This will be shown to be fulfilled in our later "idea experiment" setup. Taking complex Laplace transform on both sides of Eqn(4.31) and use $\{p(\mathbf{k}, t = 0), T(\mathbf{k}, t = 0)\}$ to be the initial condition (weird, but can't be avoided), we have

$$\begin{aligned} & \left[-izm(-iz + bk^2) + \left.\frac{\partial p}{\partial n}\right)_S k^2\right]\tilde{n}(\mathbf{k}z) + \frac{V}{T}\left.\frac{\partial P}{\partial S}\right)_n k^2\tilde{q}(\mathbf{k}z) \\ = \quad & m(-iz + bk^2)n(\mathbf{k}, t = 0) \\ = \quad & m(-iz + bk^2)\left[\left.\frac{\partial n}{\partial p}\right)_T p(\mathbf{k}, t = 0) + \left.\frac{\partial n}{\partial T}\right)_p T(\mathbf{k}, t = 0)\right] \end{aligned} \tag{4.32}$$

$$\begin{aligned} & \left[-iz + \frac{\kappa V}{T} \left.\frac{\partial T}{\partial S}\right)_n k^2\right] \tilde{q}(\mathbf{k}z) + \kappa \left.\frac{\partial T}{\partial n}\right)_S k^2 \tilde{n}(\mathbf{k}z) \\ = \quad & q(\mathbf{k}, t=0) \\ = \quad & \frac{T}{V} \left.\frac{\partial S}{\partial p}\right)_T p(\mathbf{k}, t=0) + \frac{T}{V} \left.\frac{\partial S}{\partial T}\right)_p T(\mathbf{k}, t=0) \end{aligned} \tag{4.33}$$

We can write Eqn(4.32),Eqn(4.33) in matrix form

$$\begin{bmatrix} -iz + \frac{c_S^2 k^2}{-iz+bk^2} & \frac{\frac{V}{mT} \left.\frac{\partial p}{\partial S}\right)_n k^2}{-iz+bk^2} \\ \kappa \left.\frac{\partial T}{\partial n}\right)_S k^2 & -iz + \frac{\kappa k^2}{mnc_V} \end{bmatrix} \begin{bmatrix} \tilde{n}(\mathbf{k}z) \\ \tilde{q}(\mathbf{k}z) \end{bmatrix} = \begin{bmatrix} \left.\frac{\partial n}{\partial p}\right)_T & \left.\frac{\partial n}{\partial T}\right)_p \\ \frac{T}{V} \left.\frac{\partial S}{\partial p}\right)_T & \frac{T}{V} \left.\frac{\partial S}{\partial T}\right)_p \end{bmatrix} \begin{bmatrix} p(\mathbf{k}) \\ T(\mathbf{k}) \end{bmatrix} \tag{4.34}$$

or

$$\mathbf{A} \begin{bmatrix} \tilde{n}(\mathbf{k}z) \\ \tilde{q}(\mathbf{k}z) \end{bmatrix} = \mathbf{B} \begin{bmatrix} p(\mathbf{k}) \\ T(\mathbf{k}) \end{bmatrix} \tag{4.35}$$

The solution to the matrix equation is

$$\begin{bmatrix} \tilde{n}(\mathbf{k}z) \\ \tilde{q}(\mathbf{k}z) \end{bmatrix} = \frac{1}{\det A} \mathbf{W} \begin{bmatrix} p(\mathbf{k}) \\ T(\mathbf{k}) \end{bmatrix} \tag{4.36}$$

with

$$\mathbf{W} = \begin{bmatrix} -iz + \frac{\kappa k^2}{mnc_V} & \frac{\frac{-V}{mT} \left.\frac{\partial p}{\partial S}\right)_n k^2}{-iz+bk^2} \\ -\kappa \left.\frac{\partial T}{\partial n}\right)_S k^2 & -iz + \frac{c_S^2 k^2}{-iz+bk^2} \end{bmatrix} \begin{bmatrix} \left.\frac{\partial n}{\partial p}\right)_T & \left.\frac{\partial n}{\partial T}\right)_p \\ \frac{T}{V} \left.\frac{\partial S}{\partial p}\right)_T & \frac{T}{V} \left.\frac{\partial S}{\partial T}\right)_p \end{bmatrix} \tag{4.37}$$

$$= \begin{bmatrix} (-iz + \frac{\kappa}{mnc_V} k^2) \left.\frac{\partial n}{\partial p}\right)_T - \frac{\frac{1}{m} \left.\frac{\partial p}{\partial S}\right)_n \left.\frac{\partial S}{\partial p}\right)_T k^2}{-iz+bk^2} & (-iz + \frac{\kappa}{mnc_V} k^2) \left.\frac{\partial n}{\partial T}\right)_p - \frac{\frac{1}{m} \left.\frac{\partial p}{\partial S}\right)_n \left.\frac{\partial S}{\partial T}\right)_p k^2}{-iz+bk^2} \\ -\kappa \left.\frac{\partial T}{\partial n}\right)_S \left.\frac{\partial n}{\partial p}\right)_T k^2 + (-iz + \frac{c_S^2 k^2}{-iz+bk^2}) \frac{T}{V} \left.\frac{\partial S}{\partial p}\right)_T & -\kappa \left.\frac{\partial T}{\partial n}\right)_S \left.\frac{\partial n}{\partial T}\right)_p k^2 + (-iz + \frac{c_S^2 k^2}{-iz+bk^2}) mnc_p \end{bmatrix} \tag{4.38}$$

Define *thermal diffusivity*

$$D_T = \frac{\kappa}{mnc_p} \tag{4.39}$$

and express everything in terms of $\gamma, c_S^2, \left.\frac{\partial n}{\partial T}\right)_p$. Then

$$\mathbf{W} = \begin{bmatrix} (-iz + D_T\gamma k^2)\frac{\gamma}{mc_S^2} - \frac{(1-\gamma)k^2/m}{-iz+bk^2} & (-iz + D_T\gamma k^2) \left.\frac{\partial n}{\partial T}\right)_p + \frac{c_S^2 \left.\frac{\partial n}{\partial T}\right)_p k^2}{-iz+bk^2} \\ \\ \frac{T}{n} \left.\frac{\partial n}{\partial T}\right)_p D_T\gamma k^2 + (-iz + \frac{c_S^2 k^2}{-iz+bk^2})\frac{T}{n} \left.\frac{\partial n}{\partial T}\right)_p & -\kappa(1-\gamma)k^2 + (-iz + \frac{c_S^2 k^2}{-iz+bk^2})mnc_p \end{bmatrix} \tag{4.40}$$

and

$$\begin{aligned} \det A = & \quad (-iz + \frac{c_S^2 k^2}{-iz+bk^2})(-iz + D_T\gamma k^2) - \frac{\frac{\kappa V}{mT} \left.\frac{\partial T}{\partial n}\right)_S \left.\frac{\partial p}{\partial S}\right)_n k^4}{-iz+bk^2} \\ = & \quad -iz(-iz + D_T\gamma k^2) + \frac{c_S^2 k^2(-iz)}{-iz+bk^2} + \frac{D_T\gamma c_S^2 - \frac{\kappa V}{mT} \left.\frac{\partial T}{\partial n}\right)_S \left.\frac{\partial p}{\partial S}\right)_n}{-iz+bk^2} k^4 \end{aligned} \tag{4.41}$$

but

$$\begin{aligned} \left.\frac{\partial T}{\partial n}\right)_S \left.\frac{\partial p}{\partial S}\right)_n = & \quad -\left.\frac{\partial T}{\partial n}\right)_S \left.\frac{\partial n}{\partial S}\right)_p \left.\frac{\partial p}{\partial n}\right)_S = (\gamma-1) \left.\frac{\partial T}{\partial n}\right)_p \left.\frac{\partial n}{\partial S}\right)_p mc_S^2 \\ = & \quad (\gamma-1) \left.\frac{\partial T}{\partial S}\right)_p mc_S^2 = (\gamma-1)\frac{T}{V}\frac{mc_S^2}{mnc_p} \end{aligned} \tag{4.42}$$

So

$$D_T\gamma c_S^2 - \frac{\kappa V}{mT} \left.\frac{\partial T}{\partial n}\right)_S \left.\frac{\partial p}{\partial S}\right)_n = \frac{\kappa\gamma c_S^2}{mnc_p} - \frac{\kappa c_S^2}{mnc_p}(\gamma-1) = D_T c_S^2 \tag{4.43}$$

Then

$$\det A = -iz(-iz + D_T\gamma k^2 + \frac{c_S^2 k^2}{-iz+bk^2}) + \frac{D_T c_S^2 k^4}{-iz+bk^2} \tag{4.44}$$

Up to now it is exact, the solution to the coupled equations would be just $(\det A)^{-1}\mathbf{W}$. But it is hard to see the physical picture and retrieve information from it (except later we have to take the z fixed, $\mathbf{k} \to 0$ limit in this form). In order to proceed further, we study the pole structure of $\det A$. One possibilty would be that $-iz$ goes as k^2 as in the pure diffusion case. Then we could ignore all the k^4 terms in $\det A$ and in matrix $\mathbf{W}$

$$\det A = \frac{-izc_S^2 k^2}{-iz+bk^2} + \frac{D_T c_S^2 k^4}{-iz+bk^2} = \frac{(-iz + D_T k^2)c_S^2 k^2}{-iz+bk^2} + \mathcal{O}(k^4) \tag{4.45}$$

and

$$\mathbf{W} = \begin{bmatrix} \frac{\gamma-1}{m}\frac{k^2}{-iz+bk^2} & \frac{c_S^2 \left.\frac{\partial n}{\partial T}\right)_p k^2}{-iz+bk^2} \\ & \\ \frac{\frac{T}{n}\left.\frac{\partial n}{\partial T}\right)_p c_S^2 k^2}{-iz+bk^2} & \frac{mnc_p c_S^2 k^2}{-iz+bk^2} \end{bmatrix} \tag{4.46}$$

So $(\det A)^{-1}\mathbf{W}$ around that diffusion pole is

$$\frac{\mathbf{W}}{\det A} = \begin{bmatrix} \frac{\gamma-1}{mc_S^2}\frac{1}{-iz+D_Tk^2} & \left.\frac{\partial n}{\partial T}\right)_p \frac{1}{-iz+D_Tk^2} \\ & \\ \frac{T}{n}\left.\frac{\partial n}{\partial T}\right)_p \frac{1}{-iz+D_Tk^2} & \frac{mnc_p}{-iz+D_Tk^2} \end{bmatrix} \tag{4.47}$$

On the other hand, there might be order-k poles. Look at $\det A$ in Eqn(4.44), we still want to keep to k^4 accuracy. But in order-k^2 there're only two terms

$$\det A = -z^2 + c_S^2 k^2 + \mathcal{O}(k^3) \tag{4.48}$$

we see that the pole is on the real axis, $z = \pm c_S k$, which represent a sound wave with velocity c_S. It will have a finite lifetime though if we continue to expand to the third order. Use the same trick as in calculating the quasi-particle lifetime, i.e., plug in the first solution to get the correction, we have

$$\begin{aligned} \det A = & \quad -z^2 - izD_T\gamma k^2 - iz\Big(\frac{c_S^2k^2}{-iz} - \frac{c_S^2k^2\cdot bk^2}{(-iz)^2}\Big) + \frac{-izD_Tc_S^2k^4}{(-iz)^2} \\ = & \quad -z^2 + c_Sk^2 - izk^2[D_T\gamma + b - D_T] \\ = & \quad -z^2 + c_Sk^2 - i\Gamma zk^2 + \mathcal{O}(k^4) \end{aligned} \tag{4.49}$$

where

$$\Gamma = \frac{\kappa}{mnc_p}(\frac{c_p}{c_v} - 1) + \frac{\zeta + 4\eta/3}{mn} \tag{4.50}$$

is the *sound-wave damping coefficient.* It consists of two parts, one is loss of energy through thermal conduction, the other is the diffusion of longitudinal momentum current. And

$$\mathbf{W} = \begin{bmatrix} \frac{-iz+(2\Gamma-b)k^2}{mc_S^2} & \left.\frac{\partial n}{\partial T}\right)_p (D_T\gamma + b - \Gamma)k^2 \\ & \\ \frac{T}{n}\left.\frac{\partial n}{\partial T}\right)_p (D_T\gamma + b - \Gamma)k^2 & [\kappa(\gamma-1) + (b-\Gamma)mnc_p]k^2 \end{bmatrix} + \mathcal{O}(k^3)$$

$$= \begin{bmatrix} \frac{-iz+(2\Gamma-b)k^2}{mc_S^2} & \left.\frac{\partial n}{\partial T}\right)_p D_T k^2 \\ \frac{T}{n}\left.\frac{\partial n}{\partial T}\right)_p D_T k^2 & 0 \end{bmatrix} + \mathcal{O}(k^3) \tag{4.51}$$

Notice that in the above equation k^2 terms appears with 1st order term $-iz$, they must nevertheless be kept because they are real (this is the general rule when dealing with these pole structures). When combined with the mostly real part of the denominator they will give the same order contribution to $\chi''(\mathbf{k}\omega)$.

Combining the two, we have

$$\begin{aligned} \tilde{n}(\mathbf{k}z) \quad &= \frac{\gamma-1}{mc_S^2}\frac{\mathbf{p}(\mathbf{k})}{-iz+D_Tk^2} + \left.\frac{\partial n}{\partial T}\right)_p \frac{T(\mathbf{k})}{-iz+D_Tk^2} \\ &+ \frac{-iz+(2\Gamma-b)k^2}{mc_S^2}\frac{\mathbf{p}(\mathbf{k})}{-z^2+c_S^2k^2-i\Gamma zk^2} + \left.\frac{\partial n}{\partial T}\right)_p \frac{D_Tk^2T(\mathbf{k})}{-z^2+c_S^2k^2-i\Gamma zk^2} \end{aligned} \tag{4.52}$$

$$\tilde{q}(\mathbf{k}z) = \frac{T}{n}\left.\frac{\partial n}{\partial T}\right)_p \frac{\mathbf{p}(\mathbf{k})}{-iz+D_Tk^2} + \frac{mnc_pT(\mathbf{k})}{-iz+D_Tk^2} + \frac{T}{n}\left.\frac{\partial n}{\partial T}\right)_p \frac{D_Tk^2\mathbf{p}(\mathbf{k})}{-z^2+c_S^2k^2-i\Gamma zk^2} \tag{4.53}$$

- **Linear response – System preparation:**

If we were to face the problem for the first time, we might be at a loss what to do. Clearly the approach we used in the spin diffusion problem is sound, but the mechanical handle in that problem — the external magnetic field, does not exist in this problem. How can we devise to set up an arbitary temperature and pressure field, albeit small, at $t = 0$ by applying perturbations in the Hamiltonian before $t = 0$? What seems worse is that we have to ensure it to be in local thermodynamic equilibrium *all the time* to make the comparison with hydrodynamic results valid.

The last sentence, however, embedded a clue. What Kadanoff and Martin proposed is a general correspondence principle which transforms (or rather, forms) a thermodynamic field by adding a *fictitious* perturbation term in the original Hamiltonian. The link comes from the equilibrium density matrix: $\rho = \exp\Xi/\mathrm{Tr}\exp\Xi$. For simplicity we assume it's canonical ensemble, then basically it states

$$\Big(\beta_0+\delta\beta,\mathcal{H}_0\Big) \Leftrightarrow \Big(\beta_0,(1+\frac{\delta\beta}{\beta_0})\mathcal{H}_0\Big) \tag{4.54}$$

with the density matrix invariant. Because all property averages $\langle A(\mathbf{r}t)\rangle$ would be the same, the two systems are actually *identical.* By applying the perturbation $\delta\beta\mathcal{H}_0/\beta_0$ for enough long time, we will eventually achieve what we want: a different thermodynamic field $\beta_0+\delta\beta$.

In general in a homogeneous system

$$\begin{aligned}\Xi = \quad & -\beta\Big(\sum_i \frac{(\mathbf{p}_i - m\mathbf{v})^2}{2m} + V(\mathbf{r}_1,...,\mathbf{r}_N) - \mu N\Big) \\ = \quad & -\beta\Big(\mathcal{H}_0 - \sum_i \mathbf{v}\cdot\mathbf{p}_i + \frac{1}{2}m|\mathbf{v}|^2 N - \mu N\Big)\end{aligned} \tag{4.55}$$

where μ is the chemical potential, $\mathbf{v}$ is the macroscopic velocity. When $\mathbf{v}$ is small, $\frac{1}{2}m|\mathbf{v}|^2N$ can be ignored. Then for slowly varing thermodynamic field $\delta\beta(\mathbf{r}t), \delta\mu(\mathbf{r}t), \delta\mathbf{v}(\mathbf{r}t)$

$$\delta\Xi = -\int \delta\beta(\mathbf{r}t)\left(\epsilon(\mathbf{r}t) - \mu n(\mathbf{r}t)\right)d\mathbf{r} + \beta\int \delta\mathbf{v}(\mathbf{r}t)\cdot\mathbf{j}(\mathbf{r}t)d\mathbf{r} + \beta\int \delta\mu(\mathbf{r}t)n(\mathbf{r}t)d\mathbf{r} \tag{4.56}$$

where $\epsilon(\mathbf{r}t), n(\mathbf{r}t), \mathbf{j}(\mathbf{r}t)$ now are QM operators. If we equivalence transform it to a perturbation in the Hamiltonian, then since $\delta\Xi = -\beta\delta\mathcal{H}$

$$\delta\mathcal{H} = -\int\left\{\frac{\delta T(\mathbf{r}t)}{T}\left(\epsilon(\mathbf{r}t) - \mu n(\mathbf{r}t)\right) + \delta\mathbf{v}(\mathbf{r}t)\cdot\mathbf{j}(\mathbf{r}t) + \delta\mu(\mathbf{r}t)n(\mathbf{r}t)\right\}d\mathbf{r} \tag{4.57}$$

It is more convienient to use $\delta p(\mathbf{r}t)$, the local pressure, instead of $\delta\mu(\mathbf{r}t)$

$$\delta\mu(\mathbf{r}t) = \frac{\delta p(\mathbf{r}t)}{n} - \frac{S}{nV}\delta T(\mathbf{r}t) \qquad \mu + \frac{ST}{nV} = \frac{\epsilon}{n} + \frac{p}{n} \tag{4.58}$$

$$\delta\mathcal{H} = -\int\left\{\frac{\delta T(\mathbf{r}t)}{T}q(\mathbf{r}t) + \delta\mathbf{v}(\mathbf{r}t)\cdot\mathbf{j}(\mathbf{r}t) + \frac{\delta p(\mathbf{r}t)}{n}n(\mathbf{r}t)\right\}d\mathbf{r} \tag{4.59}$$

where we had referred to Eqn(4.19). Similiar to the spin diffusion problem, the system is now prepared by perturbation

$$\delta\mathcal{H} = \begin{cases} -\int d\mathbf{r}\left\{\frac{\delta p(\mathbf{r}t)}{n}n(\mathbf{r}t) + \frac{\delta T(\mathbf{r}t)}{T}q(\mathbf{r}t) + \delta\mathbf{v}(\mathbf{r}t)\cdot\mathbf{j}(\mathbf{r}t)\right\}e^{\varepsilon t} & t \le 0 \\ \\ 0 & t > 0 \end{cases} \tag{4.60}$$

The physical meaning of this approach is so intuitive that we almost don't need any further justifications. It is O.K. as long as measurements $\langle A(\mathbf{r}, t=0)\rangle$ after the perturbation at

$t \leq 0$, equals to that of generated by *uniform equilibrium* ensemble with a little changed thermodynamic parameter $\delta p, \delta T, \delta \mathbf{v}$, which in turn can be gotten from expanding the equilibrium density matrix. This will eventually depend on whether the $k \to 0, \omega \to 0$ limit of $\chi''(\mathbf{k}\omega)$ equals to its value at $\mathbf{k} = 0, \omega = 0$. As we had said, except for long range correlated systems such as superfluid or plasmas, they are.

• Sum rules and thermodynamic derivatives

Following the procedure from Eqn(3.20) to Eqn(3.24), we have for arbitary dynamical variable A

$$\delta\tilde{A}(\mathbf{k}z) = \int \frac{d\omega}{\pi i} \frac{\chi''_{An}(\mathbf{k}z)}{\omega(\omega - z)} \frac{p(\mathbf{k})}{n} + \int \frac{d\omega}{\pi i} \frac{\chi''_{Aq}(\mathbf{k}z)}{\omega(\omega - z)} \frac{T(\mathbf{k})}{T} + \int \frac{d\omega}{\pi i} \frac{\chi''_{A\mathbf{j}}(\mathbf{k}z)}{\omega(\omega - z)} \cdot \mathbf{v}(\mathbf{k}) \qquad (4.61)$$

We are interested in A being $n(\mathbf{r}t)$, $q(\mathbf{r}t)$ or $\mathbf{j}(\mathbf{r}t)$. Obviously $\chi''_{nn}(\mathbf{r}\mathbf{r}', \omega)$, $\chi''_{nq}(\mathbf{r}\mathbf{r}', \omega)$, $\chi''_{qn}(\mathbf{r}\mathbf{r}', \omega)$, $\chi''_{qq}(\mathbf{r}\mathbf{r}', \omega)$ are all real and odd functions of ω. Because fluids are isotropic, $\chi''_{nq}(\mathbf{k}\omega) = \chi''_{nq}(k, \omega)$. It's easy to show that

$$\chi''_{nq}(k, \omega) = \chi''_{qn}(k, \omega) \qquad (4.62)$$

Eqn(4.62) is a *reciprocity* relation first discussed by Onsager. It follows from Eqn(4.61) that the response of density to a change in temperature (at constant pressure) differs only by a factor of n/T from the change in density of heat energy induced by change in pressure (at constant temperature).

The momentum current-current correlation function is of the tensor form

$$\chi''_{\mathbf{jj}}(k, \omega) = \frac{k_i k_j}{k^2} \chi''_l(k, \omega) + (\delta_{ij} - \frac{k_i k_j}{k^2}) \chi''_t(k, \omega) \qquad (4.63)$$

because we can pick our z-axis to be in the direction of $\mathbf{k}$ and the left subspace must be isotropic. l and t stands for longitudinal and transverse current autocorrelation functions. From the particle conservation equation

$$\frac{\partial}{\partial t} n(\mathbf{r}t) + \nabla \cdot \mathbf{j}(\mathbf{r}t)/m = 0, \qquad - i\omega n(\mathbf{k}\omega) + i\mathbf{k} \cdot \mathbf{j}(\mathbf{k}\omega)/m = 0$$

We have

$$\chi''_{n\mathbf{j}}(\mathbf{k}\omega) = \frac{1}{m\omega} \chi''_{\mathbf{k}\cdot\mathbf{j},\mathbf{j}}(\mathbf{k}\omega) = \frac{\mathbf{k}}{m\omega} \chi''_l(\mathbf{k}\omega)$$

$$\chi''_{nn}(\mathbf{k}\omega) = \frac{1}{m^2\omega^2}\chi''_{\mathbf{k}\cdot\mathbf{j},\mathbf{k}\cdot\mathbf{j}}(\mathbf{k}\omega) = \frac{k^2}{m^2\omega^2}\chi''_l(\mathbf{k}\omega) \tag{4.64}$$

Furthermore, $\chi''_{nn}(\mathbf{k}\omega)$ is linked to the quantity *dynamical structure factor* $S(\mathbf{k}\omega)$ through the fluctuation-dissipation theorem

$$S(\mathbf{k}\omega) = \frac{1}{2\pi n}C_{nn}(\mathbf{k}\omega) = \frac{\hbar}{2\pi n}\coth\frac{\beta\hbar\omega}{2}\chi''_{nn}(\mathbf{k}\omega) \tag{4.65}$$

$S(\mathbf{k}\omega)$ can be directly measured by thermal neutron scattering.

Similiarly, we have

$$\chi''_{\mathbf{j}q}(\mathbf{k}\omega) = \chi''_{q\mathbf{j}}(\mathbf{k}\omega) = \frac{m\omega\mathbf{k}}{k^2}\chi''_{qn}(k,\omega) \tag{4.66}$$

At $t = 0$, it follows in the same way from Eqn(3.22) that

$$A(\mathbf{k}, t = 0) = \int \frac{d\omega}{\pi}\frac{\chi''_{An}(\mathbf{k}\omega)}{\omega}\frac{p(\mathbf{k})}{n} + \int \frac{d\omega}{\pi}\frac{\chi''_{Aq}(\mathbf{k}\omega)}{\omega}\frac{T(\mathbf{k})}{T} + \int \frac{d\omega}{\pi}\frac{\chi''_{A\mathbf{j}}(\mathbf{k}\omega)}{\omega}\cdot\mathbf{v}(\mathbf{k}) \tag{4.67}$$

In our experimental setup we take $\mathbf{v}_l(\mathbf{k}) = 0$ to satisfy the initial condition of previous hydrodynamic solutions. $\mathbf{v}_t(\mathbf{k})$ can exist but the transverse current only couples to itself.

1. Take $A(\mathbf{r}t)$ to be $n(\mathbf{r}t)$, and compare Eqn(4.67) with Eqn(4.23)

   $$\left.\frac{\partial n}{\partial p}\right)_T = \lim_{k\to 0}\int \frac{d\omega}{\pi}\frac{\chi''_{nn}(\mathbf{k}\omega)}{\omega}\frac{1}{n} \tag{4.68}$$

   because as $\mathbf{k} \to 0$ $\chi''_{nn}(\mathbf{k}\omega)/\omega$ limits towards a delta function, it follows from Eqn(4.65) that

   $$\left.\frac{\partial n}{\partial p}\right)_T = \frac{1}{k_B T}\lim_{k\to 0}\int S(\mathbf{k}\omega)d\omega = \frac{1}{k_B T}S(\mathbf{k} = 0) \tag{4.69}$$

   the well-known result that the peak height of static structure factor is proportional to the isothermal compressibililty. Also,

   $$\left.\frac{\partial n}{\partial T}\right)_p = \lim_{k\to 0}\int \frac{d\omega}{\pi}\frac{\chi''_{nq}(\mathbf{k}\omega)}{\omega}\frac{1}{T} \tag{4.70}$$

2. Take $A(\mathbf{r}t)$ to be $q(\mathbf{r}t)$, then

$$\left.\frac{T}{V}\frac{\partial S}{\partial p}\right)_T = \lim_{k\to 0}\int \frac{d\omega}{\pi}\frac{\chi''_{qn}(\mathbf{k}\omega)}{\omega}\frac{1}{n} = \left.\frac{T}{n}\frac{\partial n}{\partial T}\right)_p \tag{4.71}$$

$$\left.\frac{T}{V}\frac{\partial S}{\partial T}\right)_p = \lim_{k\to 0}\int \frac{d\omega}{\pi}\frac{\chi''_{qq}(\mathbf{k}\omega)}{\omega}\frac{1}{T} = mnc_p \tag{4.72}$$

3. Take $A(\mathbf{r}t)$ to be $\mathbf{j}(\mathbf{r}t)$. We know that $\mathbf{j}(\mathbf{k}, t=0) = mn\mathbf{v}(\mathbf{k}, t=0)$, then

$$\lim_{k\to 0}\int \frac{d\omega}{\pi}\frac{\chi''_t(\mathbf{k}\omega)}{\omega} = mn \tag{4.73}$$

$$\lim_{k\to 0}\int \frac{d\omega}{\pi}\frac{\chi''_l(\mathbf{k}\omega)}{\omega} = mn \tag{4.74}$$

The second relation is in fact exact for all $\mathbf{k}$, it follows from the exact commuatation relation

$$[n(\mathbf{r}), \mathbf{j}(\mathbf{r}')] = -i\hbar\nabla(n(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')) \tag{4.75}$$

$$\chi''_{n\mathbf{j}}(\mathbf{r}\mathbf{r}', t=0) = \langle -i\hbar\nabla(n(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}'))\rangle/2\hbar \tag{4.76}$$

So

$$\begin{aligned}\chi''_{n\mathbf{j}}(\mathbf{k}, t=0) = & \quad \frac{n\mathbf{k}}{2} \\ = & \quad \int\frac{d\omega}{2\pi}\chi''_{n\mathbf{j}}(\mathbf{k}\omega) = \int\frac{\mathbf{k}d\omega}{2\pi m\omega}\chi''_l(\mathbf{k}\omega)\end{aligned} \tag{4.77}$$

and so

$$\int\frac{d\omega}{\pi}\frac{\chi''_l(\mathbf{k}\omega)}{\omega} = \int\frac{d\omega}{\pi}\frac{m^2\omega^2}{k^2}\frac{\chi''_{nn}(\mathbf{k}\omega)}{\omega} = mn \tag{4.78}$$

This is once again the frequently quoted longitudinal f-sum rule.

• Absorptive susceptibility and transport coefficients

Similiar to the procedure from Eqn(3.34) to Eqn(3.36), we have from Eqn(4.61), Eqn(4.52)

$$\begin{aligned}\chi''_{nn}(\mathbf{k}\omega) = & \quad n\omega\mathrm{Re}\frac{\tilde{n}(\mathbf{k}, w+i\varepsilon)}{p(\mathbf{k})} \\ = & \quad \frac{n\omega}{mc_S^2}\frac{(\gamma-1)D_Tk^2}{\omega^2+(D_Tk^2)^2} + \frac{n\omega}{mc_S^2}\frac{\Gamma c_S^2k^4 - D_T(\gamma-1)(\omega^2-c_S^2k^2)k^2}{(\omega^2-c_S^2k^2)^2+(\Gamma\omega k^2)^2}\end{aligned} \tag{4.79}$$

$$\chi''_{qq}(\mathbf{k}\omega) = T\omega\mathrm{Re}\frac{\tilde{q}(\mathbf{k}, w + i\varepsilon)}{T(\mathbf{k})} = \frac{mnc_pTD_Tk^2\omega}{\omega^2 + (D_Tk^2)^2} \tag{4.80}$$

$$\chi''_{nq}(\mathbf{k}\omega) = T\omega\mathrm{Re}\frac{\tilde{n}(\mathbf{k}, w + i\varepsilon)}{T(\mathbf{k})} = T\left.\frac{\partial n}{\partial T}\right)_p \left[\frac{D_Tk^2\omega}{\omega^2 + (D_Tk^2)^2} - \frac{D_Tk^2\omega(\omega^2 - c_S^2k^2)}{(\omega^2 - c_S^2k^2)^2 + (\Gamma\omega k^2)^2}\right] \tag{4.81}$$

Lastly, from Eqn(4.15),Eqn(4.61)

$$\chi''_t(\mathbf{k}\omega) = \omega\mathrm{Re}\frac{\tilde{\mathbf{j}}_t(\mathbf{k}, \omega + i\varepsilon)}{\mathbf{v}_t(\mathbf{k})} = \frac{\eta k^2\omega}{\omega^2 + \left(\frac{\eta k^2}{mn}\right)^2} \tag{4.82}$$

An important point is in order: remember that in deriving Eqn(4.52),Eqn(4.53) the method we used is to pick out order-k and order-k^2 poles in z for each chosen wave-vector $\mathbf{k}$. We then calculate the residue, i.e., coefficient on these simple poles of z which, at there are functions of mixed $\mathbf{k}, z$. We then superimpose the two pole structures to get Eqn(4.52), Eqn(4.53). However, why do we choose that specific form for these residue functions and why, in the sound propagation case, do we use $-i\Gamma zk^2$ as the imaginary part in the denominator? Why can't we replace the extra $-iz$'s by its value at the pole in terms of k? The answer is that although other forms will still give the correct residue on the pole, they would lead to wrong $\mathbf{k} \to 0$ behaviour when z is fixed. That limit will be used later to derive transport coefficients, as from the linear response side we must take $\lim_{k\to 0}$ first to get closed expressions. Although soon we'll use Eqn(4.79), Eqn(4.80), Eqn(4.81), which are derived from Eqn(4.52),Eqn(4.53), to show that, keep in mind that the sequence should really be reversed. In practice, we should use the *exact expression* Eqn(4.44),Eqn(4.40) to show the $\lim_{\omega\to 0}\lim_{k\to 0}$ identity:

$$\begin{aligned} \text{some transport coefficient} &= \lim_{\omega\to 0}\lim_{k\to 0}\frac{\omega^\alpha}{k^\beta}\mathrm{Re}\frac{\tilde{A}(\mathbf{k}, \omega + i\varepsilon)}{b(\mathbf{k})} \\ (\textit{from linear response}) &= \int dtd\mathbf{r}\langle\{A(\mathbf{r}t), B(\mathbf{0}0)\}\rangle \end{aligned} \tag{4.83}$$

and then adjust our residue expression in Eqn(4.52), Eqn(4.53) to match that (they happen to be correct now, as they are the form from Kadanoff and Martin's paper). Then the formulas will be better *approximations* for the exact $(\det A)^{-1}\mathbf{W}$, as they have the correct pole structure and take the correct limits too. Please check that all the following limits can be in fact directly derived from Eqn(4.44),Eqn(4.40), when doing so please remember keeping different orders of k for real and imaginary parts. Especially, in the case of Eqn(4.92), expansion must be kept to k^4 accuracy. It is always safe to check with Eqn(4.44),Eqn(4.40), don't rely too much on the nice looking Eqn(4.52),Eqn(4.53).

In entirely the same fashion of deriving the spin diffusion coefficient from

$$D_M\chi_{MM} = \lim_{\omega\to 0}\Big(\lim_{k\to 0}\frac{\omega}{k^2}\chi''_{MM}(\mathbf{k}\omega)\Big)$$

to

$$D_M\chi_{MM} = \frac{1}{4k_BT}\int dtd\mathbf{r}\Big\langle\Big\{\mathbf{J}^M_x(\mathbf{r}t),\mathbf{J}^M_x(\mathbf{00})\Big\}\Big\rangle$$

(Eqn(3.34) to Eqn(3.36)), we have for the same *thermal* diffusion structure Eqn(4.80)

$$\begin{aligned} mnc_pTD_T = &\quad \lim_{\omega\to 0}\Big(\lim_{k\to 0}\frac{\omega}{k^2}T\omega\mathrm{Re}\frac{\tilde{q}(\mathbf{k},\omega+i\varepsilon)}{T(\mathbf{k})}\Big) \\ = &\quad \lim_{\omega\to 0}\Big(\lim_{k\to 0}\frac{\omega}{k^2}\chi''_{qq}(\mathbf{k}\omega)\Big) \\ = &\quad \frac{1}{4k_BT}\int dtd\mathbf{r}\langle\{\mathbf{j}^q_x(\mathbf{r}t),\mathbf{j}^q_x(\mathbf{00})\}\rangle \\ = &\quad \kappa T \end{aligned} \tag{4.84}$$

where $\mathbf{j}^q$ is the *heat current* operator defined by

$$\mathbf{j}^q(\mathbf{r}t) = \frac{\partial}{\partial t}\epsilon(\mathbf{r}t) - (p+\epsilon)\mathbf{v}(\mathbf{r}t) = \mathbf{j}^\epsilon(\mathbf{r}t) - (p+\epsilon)\mathbf{v}(\mathbf{r}t) \tag{4.85}$$

However, according to Eqn(4.79) (or rather, Eqn(4.44) and Eqn(4.40))

$$\begin{aligned} \lim_{\omega\to 0}\lim_{k\to 0}\frac{\omega}{k^2}\chi''_{nn}(\mathbf{k}\omega) = &\quad \lim_{\omega\to 0}\lim_{k\to 0}\frac{\omega}{k^2}\Big(n\omega\mathrm{Re}\frac{\tilde{n}(\mathbf{k},\omega+i\varepsilon)}{p(\mathbf{k})}\Big) \\ = &\quad \frac{n}{mc_S^2}((\gamma-1)D_T - D_T(\gamma-1)) \\ = &\quad 0 \end{aligned} \tag{4.86}$$

and

$$\begin{aligned} \lim_{\omega\to 0}\lim_{k\to 0}\frac{\omega}{k^2}\chi''_{nq}(\mathbf{k}\omega) = &\quad \lim_{\omega\to 0}\lim_{k\to 0}\frac{\omega}{k^2}\Big(T\omega\mathrm{Re}\frac{\tilde{n}(\mathbf{k},\omega+i\varepsilon)}{T(\mathbf{k})}\Big) \\ = &\quad T\left.\frac{\partial n}{\partial T}\right)_p(D_T - D_T) \\ = &\quad 0 \end{aligned} \tag{4.87}$$

So there must be

$$0 \equiv \int dtd\mathbf{r} \langle \{ \mathbf{v}_x(\mathbf{r}t), \mathbf{v}_x(\mathbf{0}0) \} \rangle \equiv \int dtd\mathbf{r} \langle \{ \mathbf{v}_x(\mathbf{r}t), \mathbf{j}^q_x(\mathbf{0}0) \} \rangle \tag{4.88}$$

so it doesn't matter whether we use $\mathbf{j}^q$ or $\mathbf{j}^\epsilon$ in Eqn(4.84)

$$\kappa = \frac{1}{4k_B T^2} \int dtd\mathbf{r} \langle \{ \mathbf{j}^q_x(\mathbf{r}t), \mathbf{j}^q_x(\mathbf{0}0) \} \rangle = \frac{1}{4k_B T^2} \int dtd\mathbf{r} \langle \{ \mathbf{j}^\epsilon_x(\mathbf{r}t), \mathbf{j}^\epsilon_x(\mathbf{0}0) \} \rangle \tag{4.89}$$

In practice we always use $\mathbf{j}^\epsilon$.

From Eqn(4.82) we see that

$$\eta = \lim_{\omega \to 0} \lim_{k \to 0} \frac{\omega}{k^2} \chi''_t(\mathbf{k}\omega) \tag{4.90}$$

Take $\mathbf{k}$ to be in the z-direction and the tranverse current in x, then similiar to Eqn(3.36)

$$\begin{aligned} \eta = & \frac{1}{4k_B T} \lim_{\omega \to 0} \lim_{k \to 0} \frac{1}{k^2} \int dtd\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega t} \langle \{ \mathbf{k} \cdot \vec{\tau}_x(\mathbf{r}t), \mathbf{k} \cdot \vec{\tau}_x(\mathbf{0}0) \} \rangle \\ = & \frac{1}{4k_B T} \int dtd\mathbf{r} \langle \{ \tau_{xz}(\mathbf{r}t), \tau_{xz}(\mathbf{0}0) \} \rangle \end{aligned} \tag{4.91}$$

i.e., by integrating the correlation function of instantaneous shear stress we can get the shear viscosity.

After some (hard) work struggling with Eqn(4.79) (or rather, Eqn(4.44), Eqn(4.40)) to the k^4 order, we can show that the bulk viscosity ζ can be gotten from

$$\begin{aligned} \zeta + \frac{4}{3}\eta = bmn = & \lim_{\omega \to 0} \left(\lim_{k \to 0} \frac{m^2 \omega^3}{k^4} n\omega \mathrm{Re} \frac{\tilde{n}(\mathbf{k}, \omega + i\varepsilon)}{p(\mathbf{k})} \right) \\ = & \lim_{\omega \to 0} \left(\lim_{k \to 0} \frac{m^2 \omega^3}{k^4} \chi''_{nn}(\mathbf{k}\omega) \right) \\ = & \lim_{\omega \to 0} \left(\lim_{k \to 0} \frac{\omega}{k^2} \chi''_l(\mathbf{k}\omega) \right) \\ = & \frac{1}{4k_B T} \int dtd\mathbf{r} \langle \{ \tau_{zz}(\mathbf{r}t) - p, \tau_{zz}(\mathbf{0}0) - p \} \rangle \end{aligned} \tag{4.92}$$

...and now that little thing of which Gregor had dreamed during so many sleepless nights had come to pass. He stood at his gate of his own home, holding his son by the hands. This was

all life had left to him, all that for a little longer gave him kinship with the earth and with the spacious world which lay glittering under the chilly sun.

— from *The Quiet Don* by Mikhail Sholokhov.