Notes 2 - Section 2

→ Hydrodynamic Equations and Correlation Functions, I

c.f. Kadanoff and Martin, posted, systematics
Landau & Lifshitz; Statistical Phys. Fluctuations
D Forster "Hydrodynamic Fluctuations, Broken Symmetry, Correlation Functions".

Point of Kubo-ology:

- Linear response and transport coefficient for weakly non-equilibrium systems linked to equilibrium correlation function.

- Diffusion ~~&~~ scattering, memory.

More generally:

→ Nonequilibrium behavior of interest, but hard (huge # DOFs)

→ can leverage non-equilibrium insights by considering slow variation in space, time.

e.g. fluid mechanics (smooth)
(reduced d-o-f)

but where from:
- transport coefficients (i.e. ν)
- thermodynamic quantities ?

Recall:

- considered linear response, and weak (stochastic) scattering of and cf:

- Two classic Kubo results:

$$\underline{\underline{\sigma}}(\omega) = \int_0^\infty e^{i\omega\tau} \frac{\beta}{\underline{\underline{V}}} \langle \underline{\tilde{J}}(\Gamma)\, \underline{\tilde{J}}(\Gamma(-\tau)) \rangle_\Gamma$$

→ conductivity as F.T. of eq'brm current correlation

$$D = \int_0^\infty d\tau \, \langle \tilde{v}(0)\, \tilde{v}(\tau) \rangle$$

→ Diffusion as integral of velocity correlation

$\boxed{\text{Know!}}$

⇒ Non-perturbative approach to transport

Points: (extending Kubo ideology)

→ time dependent correlation functions are useful tool for investigating (theoretical) behavior of nonequilibrium systems.

→ correlation functions contain all relevant info when deviation from equilibrium is small.

correlation ↔ response $\chi(k,\omega)$

⇒ Hence the strong focus on correlation functions!

⇒ Hydrodynamic equations and correlation functions

→ collective behavior (modes)

→ not an expansion in interactions, collisions.
(asymptotic $(k, \omega \to 0)$), not perturbative).
→ leverage is $\begin{matrix} k \\ \omega \end{matrix} \to 0$.

Thrust here:

→ How use hydrodynamic equations to understand correlation?
→ How relate correlation, transport, susceptibility.

N.B. Shift in focus:

Kinetics Boltzmann Equation (f) μ-scopics	→	Hydrodynamics Fluid equations (macro-correln. $\langle nn \rangle$) Macroscopics.

Simple examples:

ⓐ – spin magnetization. (fluid)

Show:
magnetization,
→ Correlation function ↔ {thermodynamic response; transport coeffs}

ⓑ – Single component fluid (linear dynamics).

P.T.: [Correlation function (spectra) easily measureable]

→ Spin Diffusion

– Hydro Description

Fluid — (uncharged, spin 1/2
(particles interact by velocity, spin indep force
(spin quantization direction

order parameter

$\underline{M}(\underline{x},t) \equiv$ magnetization (spin) at $(\underline{r},t)$. $= n_{up}^{(x,t)} S_{1/2} - n_{down} S_{-1/2}$

Global cons Law

$$\frac{d}{dt}\int d^3x \; \underline{M}(\underline{x},t) = 0.$$

Presumes direction

– total magnetization conserved

Local Balance

M scalar.

$$\frac{\partial \underline{M}(\underline{x},t)}{\partial t} + \underline{\nabla}\cdot\underline{J}_M = 0$$

$\underline{J}_M$: magnetization current.

Conserved order parameter

($\underline{M}(\underline{x},t)$ can change locally).

can relate to particles! [macro-micro link]

$$\underline{M}(\underline{x},t) = \sum_{r} \gamma\, \underline{S}_r(t)\, \delta(\underline{r}-\underline{r}_r(t))$$

$$\underline{J}_M(\underline{x},t) = \sum_{r} \gamma\, \frac{\underline{S}_r(t)}{2M} \left\{ \underline{p}_r(t),\, \delta(\underline{r}-\underline{r}_r(t)) \right\}$$

$$\xrightarrow{\text{classically}} \sum_{r} \gamma\, \frac{\underline{S}_r(t)}{2m}\, \underline{p}_r(t)\, \delta(\underline{r}-\underline{r}_r(t))$$

QM operators.

$$\{A, B\} = AB + BA$$ symmetric

Now, how close?

→ if properties vary slowly; constitutive relation.

$$\boxed{\langle \underline{J}_M(\underline{x},t) \rangle = -D\, \nabla \langle \underline{M}(\underline{x},t) \rangle}$$

- valid for slow dependence
→ response to non-eq'brm.

$$\langle J_M \rangle = -D\, \underline{\nabla} \langle M \rangle + \cdots$$

$$\boxed{\text{what is } D\ ??}$$

Of course,

$$\frac{\partial \langle M \rangle}{\partial t} + \underline{\nabla} \cdot \langle \underline{J}_M \rangle = 0$$

$$\langle \underline{J}_M \rangle = - D \, \underline{\nabla} \langle M \rangle$$

⇒ Magnetization diffusion eqn.:

$$\boxed{\frac{\partial \langle M \rangle}{\partial t} = D \nabla^2 \langle M \rangle.}$$

[weak deviation from eqbm.

N.B. → compare kinematic waves

$$\partial_t \rho + \partial_x \Gamma(\rho) - \nu \partial_x^2 \rho = 0$$

$$\rho V(\rho) \rightarrow \text{NL.}$$

$$\partial_t \rho + c(\rho) \partial_x \rho - \nu \partial_x^2 \rho = 0$$

fluid dynamics

diffn

$$\frac{\partial c(\rho)}{\partial \rho} > 0 \rightarrow \text{shock}.$$

can be strongly NL

Can understand:

$$\underline{J} = -D\,\underline{\nabla} M$$

as lowest order expansion of $\underline{J}$

$$\underline{J} = -\Gamma \nabla \frac{\delta F}{\delta M}$$

$$F = \alpha \frac{M^2}{2} + b\,\frac{M^4}{4}$$

so

$$\underline{J} = -\Gamma \nabla \left(\alpha M + b M^3 + \cdots \right)$$

$$D = \Gamma \alpha$$

if $\alpha < 0$, $D < 0$!?

$$F = \alpha \frac{M^2}{2} + b\,\frac{M^4}{4} + c\,\frac{(\nabla M)^2}{2}$$

$D < 0$

positive hyper-diffn.

How deviate from equilibrium ??

→ external magnetic field H (same direction) ⇒ induce deviation

$$H(\underline{x},t) = H(\underline{x})\, e^{t} \quad t<0$$
$$= 0 \quad t>0$$

causality

$$\langle M(\underline{x}) \rangle = \chi H(\underline{x})$$

spin susceptibility (static) (thermo. quantity)

$$\boxed{\chi = \left.\frac{\partial M}{\partial H}\right|_{H=0}}$$

response

so

— H on $(t<0)$ $\quad M = \chi H$

H off: [redacted]

$$\frac{\partial \langle M \rangle}{\partial t} = D \nabla^2 \langle M \rangle$$ → diffusive relaxation

To represent relaxation:

$$M(\underline{k}, z) = \int d^3x \, e^{-i\underline{k}\cdot\underline{x}} \int_0^\infty dt \, e^{izt} \langle M(\underline{x},t)\rangle$$

Laplace transform $\rightarrow$ direction of time

z in uhp $(z + i\epsilon)$

so

$$\int d^3x \, e^{-ik\cdot x} \int_0^\infty dt \, e^{izt} \left[\frac{\partial\langle M\rangle}{\partial t} - D \nabla^2 \langle M\rangle \right] = 0$$

$$0 = \left(-iz + k^2 D\right) M(\underline{k}, z) - \int d\underline{r} \, e^{-ik\cdot x} \langle M(\underline{x}, 0)\rangle$$

cup.

but $t < 0$ consideration,

$$\langle M(\underline{x}, 0)\rangle = \chi H(\underline{x})$$

so

$$\boxed{M(k, z) = \frac{\chi H(k)}{-iz + k^2 D}}$$

can use for correlation

gives order parameter.

So $\rightarrow$ have laid foundations of hydrodynamic description.

Now:

B.) Correlation Fctn. Description

$$H = H_0 + \delta H$$

$H \downarrow$ Hamiltonian

$\delta H \hookrightarrow = -\int d\underline{x}\, H(\underline{x},t)\, M(\underline{x},t)$

so, for any $A(\underline{x},t)$ $\downarrow$ opr.

commutator $\downarrow i\partial_t A + [A,H] = dA/dt$

$$\boxed{\delta\langle A\rangle = -i\int_{-\infty}^{t} dt' \,\langle[A(\underline{x},t),\, \delta H(\underline{x},t)]\rangle_{eq}}$$

i.e. $\dfrac{\partial A}{\partial t} = -\{A, \delta H\}_{PB.}$ QM. classical

Then, for induced magnetization:

$\langle M(\underline{x},t)\rangle \rightarrow \delta\langle M\rangle$

$$\delta\langle M(\underline{x},t)\rangle = i\int_{-\infty}^{t} dt'\, e^{\epsilon t'}\int dx\, H(\underline{x}')\langle[M(\underline{x},t), M(\underline{x}',t')]\rangle_{eq}$$

$t \leq 0$

* What is χ'', χ.

and indirect meas'n -

$$\boxed{\delta\langle M(\underline{x},t)\rangle = i\int_{-\infty}^{0} dt'\, e^{\epsilon t'} \int d\underline{x}'\, H(\underline{x}')\,\langle[M(\underline{x},t), M(\underline{x}',t')]\rangle_{eq}}$$

$t \geq 0$

- Now, need representation of eq'brm commutator.

- as space, time translation invariant, can define dynamic susceptibility (absorptive part) by

defines χ'' (FDT)

$$\langle[M(\underline{x},t), M(\underline{x}',t')]\rangle_{eq}$$

$$= \int \frac{d\omega}{\pi} \int \frac{d\underline{k}}{(2\pi)^3}\, \chi''(\underline{k},\omega)\, e^{i\underline{k}\cdot(\underline{x}-\underline{x}')}\, e^{-i\omega(t-t')}$$

$[\delta M = \chi H]$

physically meaningful defn ? $\Rightarrow$ dynamic susceptibility (absorptive part) $\rightarrow$ [must be linked to diffn.]

Aside: Dynamic susceptibility and Kramers - Kronig relation

Susceptibility:

Here, $\underline{M}(k,\omega) = \chi(k,\omega)\, H(k,\omega)$

- response function

$\underline{P} = \chi \underline{E}$, $\quad \epsilon = 1 + 4\pi\chi$,

- ex. $\underline{D}_{k,\omega} = \epsilon(k,\omega)\, \underline{E}_{k,\omega}$

$\epsilon(k,\omega) \downarrow$ dielectric fctn.

i.e. $\underline{E}$ applied, get displacement $\underline{D}$

- ϵ is complex:

$$\epsilon = \underbrace{\epsilon_r(k,\omega)}_{\text{screening}} + i\, \underbrace{\epsilon_{Im}(k,\omega)}_{\substack{\text{absorptive} \\ \text{(dissipn)}}}$$

Poynting Thm:

$$\partial_t \left(\frac{\epsilon_r E^2}{2} + \frac{H^2}{2} \right) + \nabla \cdot \underset{\text{Poynting vector}}{\underline{S}}$$

$$+ \underbrace{\omega\, \epsilon_{Im} \frac{|\underline{E}|^2}{2}}_{\text{absorption}} = 0$$

How relate ϵ_r, ϵ_{Im}?

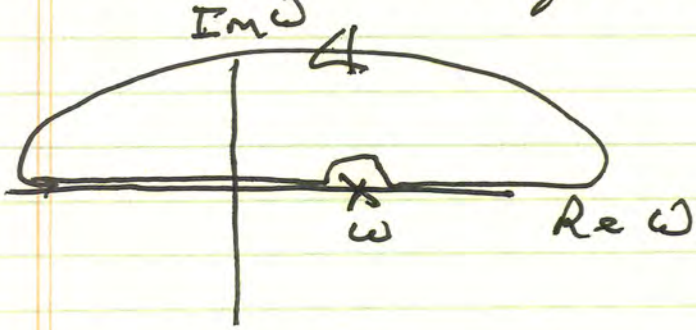
→ Kramers-Kronig Relation:

$$\epsilon_r(k,\omega) = \frac{1}{\pi} P\int_{-\infty}^{+\infty} \frac{\epsilon_{Im}(\omega')}{\omega'-\omega}\, d\omega'$$

$$\epsilon_{Im}(k,\omega) = -\frac{P}{\pi}\int_{-\infty}^{+\infty} \frac{\epsilon_r(k,\omega')}{\omega'-\omega}\, d\omega'$$

$\epsilon \leftrightarrow \chi$ generally.

If ϵ analytic in UHP:



$$\oint \left[\frac{\epsilon(\omega')}{(\omega'-\omega)}\right] d\omega' = 0.$$

so

$$0 = P\int_{-\infty}^{+\infty} \frac{\epsilon(\omega')}{\omega'-\omega}\, d\omega' - i\pi\,\epsilon(\omega)$$

As,

$$\frac{1}{\omega'-\omega} = P\frac{1}{\omega'-\omega} - i\pi\delta(\omega'-\omega)$$

so

$$i\pi\left(\epsilon_r + i\epsilon_{IM}\right)[(\omega)]$$

$$= P\int_{-\infty}^{+\infty} \frac{\left(\epsilon_r(\omega') + i\,\epsilon_{IM}(\omega')\right)}{(\omega'-\omega)}\, d\omega'$$

$\Rightarrow$

$$\epsilon_{IM}(\omega) = \frac{-1}{\pi} P\int_{-\infty}^{+\infty} \frac{\epsilon_r(\omega')}{\omega'-\omega}\, d\omega'$$

$$\epsilon_{re}(\omega) = \frac{1}{\pi} P\int_{-\infty}^{+\infty} \frac{\epsilon_{IM}(\omega')}{\omega'-\omega}\, d\omega'$$

and generalizes to any;

$\chi_{Re}(\omega)$, $\chi_{IM}(\omega)$. (analytic in UHP)

K–K Relation:

– founded on causality $\Rightarrow \begin{cases} \text{time} \\ \text{frequency} \end{cases}$

→ dissipation – reaction linked by phase ⇒ 1 determines other

so

Now returning to Magnetization doing the time integrals: (using χ'')

$$\langle M(\underline{x},t)\rangle = \int \frac{d\underline{k}}{(2\pi)^3} H_0(\underline{k})\, e^{i\underline{k}\cdot\underline{x}} \int \frac{d\omega}{\pi} \frac{\chi''(k,\omega)}{\omega} e^{-i\omega t}$$

$t \geq \infty$

and

$$\langle M(\underline{x},t)\rangle = \int \frac{d\underline{k}}{(2\pi)^3} H_0(\underline{k})\, e^{i\underline{k}\cdot\underline{x}} \int \frac{d\omega}{\pi} \frac{\chi''(k,\omega)}{\omega}$$

$t \leq 0$

And,

$$M(\underline{k}, z) = \int d\underline{x}\, e^{-i\underline{k}\cdot\underline{x}} \int_0^\infty dt\, e^{izt} \langle M(\underline{x}, t)\rangle$$

but induced magn:

$$\langle M(\underline{x},t)\rangle = i\int_{-\infty}^{0} dt'\, e^{\epsilon t'} \int d\underline{x}'\, H(\underline{x}')\ \int \frac{d\omega}{\pi} \int \frac{d\underline{k}}{(2\pi)^3}\, \chi''(\underline{k},\omega)\, e^{i\underline{k}\cdot(\underline{x}-\underline{x}')}\, e^{-i\omega(t-t')}$$

$(t \geq 0)$

so

$$\boxed{M(\underline{k}, z) = \int \frac{d\omega}{\pi i} \frac{\chi''(\underline{k},\omega)}{\omega(\omega - z)} H_0(\underline{k})}$$

used rotational inv.. $\underline{k} \to k$

and can use: $(z \to \omega + i\epsilon)$

$$\lim_{\epsilon \to 0} \frac{1}{\omega' - \omega - i\epsilon} = P\frac{1}{\omega' - \omega} + i\pi\delta(\omega - \omega')$$

so (taking $H_0(k)$ real)

$$\mathrm{re}\left[M(\underline{k}, \omega + i\epsilon)\right] = \frac{\chi''(k,\omega)}{\omega} H_0(\underline{k})$$

so

$$\mathrm{re}\left[\frac{M(k,\omega)}{H_0(k)}\right] = \frac{\chi''(k,\omega)}{\omega}$$

but have:

$$M(k,z) = \frac{\chi H_0(k)}{-iz + Dk^2}$$

so

$$\chi''(k,\omega) = \omega\, \mathrm{re}\left[\frac{M(k,\omega)}{H_0(k)}\right]$$

$$\chi'' = \omega \frac{\chi D k^2}{\omega^2 + (k^2 D)^2}$$

gives relation between dynamic susceptibility and transport coefficient(s): D, χ

elt' kubo: Resp — Transport

Important

$$\boxed{\chi''(k,\omega) = \left[\frac{\omega \chi k^2 D}{\omega^2 + (k^2 D)^2}\right]}$$

[physically meaningful]

key → defines dynamic suscept.

χ'' expression contains a lot of info! 16.
χ' via K-K relation.
And can specialize to:

$$\boxed{\begin{array}{l} \chi''(k,\omega) \cong \omega\chi_0/Dk^2 \\ \chi''(k,\omega) \cong \chi_0 k^2 D/\omega \end{array}}$$

, $\omega \ll k^2 D$ (low frequency)

, $\omega \gg k^2 D$ (high frequency)

Finally, deduce commutator / correlation function:

$$\langle [M(\underline{x},t), M(x',t')] \rangle_{eq}$$

$$= \int \frac{d\omega}{\pi} \int \frac{dk}{(2\pi)^3} \chi''(k,\omega)\, e^{ik\cdot(x-x')}\, e^{-i\omega(t-t')}$$

$$\chi'' = \frac{\omega\chi_0 k^2 D}{\omega^2 + (k^2 D)^2}$$

pole at $\quad \omega = -ik^2 D$

$\Rightarrow$

$$\langle M(\underline{x},t), M(\underline{x}',t') \rangle_{eq}$$

$$= -i\chi D \int \frac{dk}{(2\pi)^3} k^2 e^{ik(\underline{x}-\underline{x}')} e^{-k^2 D(t-t')}$$

<u>diffusive</u> <u>relaxation</u>!

$\Downarrow$

<u>relaxation</u>

→ Physically meaningful result for commutator correlator

Magnetization correlation relaxes diffusively.

→ Links correlator to susceptibility and diffusion.