Tutorial sheet 4

The exercise marked with a star is homework.

Discussion topics:

– Phase-space density of a classical many-particle system and quantum mechanical density operator, and their time evolution. Classical and quantum-mechanical Liouville operators.
– Linear response function and generalized susceptibility; Kubo formula.

11. Liouville (super)operator in quantum mechanics

Consider a quantum mechanical system governed by the Hamilton operator $\hat{H}$ acting on the Hilbert space $\mathscr{H}$. The operators $\hat{O}(t)$ acting on the kets of $\mathscr{H}$ actually form themselves a vector space, called *Liouville space* $\mathscr{E}_{\mathrm{L}}$, and their evolution is governed by the *Liouville (super)operator* $\hat{\hat{\mathcal{L}}}$, according to

$$\frac{\mathrm{d}\hat{O}(t)}{\mathrm{d}t} = \mathrm{i}\,\hat{\hat{\mathcal{L}}}\hat{O}(t) \equiv \frac{1}{\mathrm{i}\hbar}\big[\hat{O}(t),\hat{H}\big].$$

The problem in the following is to investigate the hermiticity of $\hat{\hat{\mathcal{L}}}$ for various inner products on $\mathscr{E}_{\mathrm{L}}$. Hereafter, $\hat{A}$ and $\hat{B}$ denote two vectors of $\mathscr{E}_{\mathrm{L}}$ — i.e. two operators on $\mathscr{H}$ —, $\hat{O}^\dagger$ is the Hermitian conjugate[1] (for the inner product on $\mathscr{H}$) of $\hat{O}$, and Tr the trace. In questions **ii.** and **iii.** $Z(\beta)$ denotes the canonical partition function associated to the Hamilton operator $\hat{H}$ at an inverse temperature β.

Hint: Only very short calculations are needed.

i. Consider the (Hilbert–Schmidt) product $\langle\hat{A},\hat{B}\rangle \equiv \mathrm{Tr}\big(\hat{A}^\dagger\hat{B}\big)$. Is the Liouville operator $\hat{\hat{\mathcal{L}}}$ Hermitian for this product?

ii. Same question for $\langle\hat{A},\hat{B}\rangle \equiv \frac{1}{2}\mathrm{Tr}\left[\frac{\mathrm{e}^{-\beta\hat{H}}}{Z(\beta)}\big(\hat{A}^\dagger\hat{B}+\hat{B}\hat{A}^\dagger\big)\right]$ (symmetric correlation function).

iii. Same question for $\langle\hat{A},\hat{B}\rangle \equiv \int_0^\beta \mathrm{Tr}\left[\frac{\mathrm{e}^{-\beta\hat{H}}}{Z(\beta)}\,\mathrm{e}^{\lambda\hat{H}}\hat{A}^\dagger\,\mathrm{e}^{-\lambda\hat{H}}\hat{B}\right]\mathrm{d}\lambda$ (canonical correlation function).

12. Nonlinear response

We want to investigate the lowest-order nonlinear correction to the response of the observable $\hat{B}$ of a system at equilibrium to an external perturbation $-f(t)\hat{A}$. Writing

$$\big\langle\hat{B}_{\mathrm{I}}(t)\big\rangle_{\mathrm{n.eq.}} = \big\langle\hat{B}\,\big\rangle_{\mathrm{eq.}} + \int\chi^{(1)}_{BA}(t,t')f(t')\,\mathrm{d}t' + \iint\chi^{(2)}_{BA}(t,t',t'')f(t')f(t'')\,\mathrm{d}t'\,\mathrm{d}t'' + \mathcal{O}(f^3),$$

where the integrals run over $\mathbb{R}$, show that the second-order term involves the response function

$$\chi^{(2)}_{BA}(t,t',t'') = \frac{1}{(\mathrm{i}\hbar)^2}\,\Theta(t-t')\,\Theta(t'-t'')\,\Big\langle\Big[\big[\hat{B}_{\mathrm{I}}(t),\hat{A}_{\mathrm{I}}(t')\big],\hat{A}_{\mathrm{I}}(t'')\Big]\Big\rangle_{\mathrm{eq.}}.$$

*13. Linearized Navier–Stokes equation and shear viscosity

For this exercise you actually need no result or knowledge from the lectures. Yet as hinted at by the comment at the very end, there is a relationship to (classical) linear response theory.

The dynamics of a simple one-component fluid subject to an external force field (e.g. a gravity field) is governed by the Navier–Stokes equation

$$m\mathscr{n}(t,\vec{r})\left[\frac{\partial\vec{\mathsf{v}}(t,\vec{r})}{\partial t} + \big[\vec{\mathsf{v}}(t,\vec{r})\cdot\vec{\nabla}\big]\vec{\mathsf{v}}(t,\vec{r})\right] = -\vec{\nabla}\mathcal{P}(t,\vec{r}) + \eta\triangle\vec{\mathsf{v}}(t,\vec{r}) + \left(\zeta+\frac{\eta}{3}\right)\vec{\nabla}\big[\vec{\nabla}\cdot\vec{\mathsf{v}}(t,\vec{r})\big] + \mathscr{n}(t,\vec{r})\vec{F}(t,\vec{r}),$$

[1] a.k.a. adjoint.

where m denotes the mass of the particles constituting the fluid and $\vec{F}$ the external force on one such particle. The (constant) coefficients ζ, η are the shear and bulk viscosities, while the fields n, $\vec{v}$, and $\mathcal{P}$ are respectively the particle number density, flow velocity, and pressure.

It is assumed that the latter are small deviations from uniform values n_0, $\vec{v}_0 = \vec{0}$, and $\mathcal{P}_0$ corresponding to a motionless fluid, for instance $n(t,\vec{r}) = n_0 + \delta n(t,\vec{r})$ with $|\delta n(t,\vec{r})| \ll n_0$.

i. Linearize first the Navier–Stokes equation to first order in the small quantities and take the curl of the result. This should give you an evolution equation ($\mathcal{E}$) — comprising three terms involving m, n_0, η, and $\vec{G}(t,\vec{r}) \equiv \vec{\nabla} \times \vec{F}(t,\vec{r})$ — for the *vorticity* $\vec{\omega}(t,\vec{r}) \equiv \vec{\nabla} \times \vec{v}(t,\vec{r})$.[2] Which generic type of equation do you recognize?

ii. We introduce Fourier transforms of the remaining fields in ($\mathcal{E}$) with respect to both space and time:[2]

$$\tilde{\vec{\omega}}(\omega,\vec{k}) \equiv \int \vec{\omega}(t,\vec{r})\, e^{i(\omega t - \vec{k}\cdot\vec{r})}\, dt\, d^3\vec{r} \quad \text{and} \quad \tilde{\vec{G}}(\omega,\vec{k}) \equiv \int \vec{G}(t,\vec{r})\, e^{i(\omega t - \vec{k}\cdot\vec{r})}\, dt\, d^3\vec{r}.$$

Show that the evolution equation ($\mathcal{E}$) leads to the simple algebraic relation

$$\tilde{\vec{\omega}}(\omega,\vec{k}) = \sigma(\omega,\vec{k})\tilde{\vec{G}}(\omega,\vec{k}), \tag{1}$$

where the "admittance" $\sigma(\omega,\vec{k})$ depends, besides its variables, on the parameters m, n_0, and η.

iii. Separate $\sigma(\omega,\vec{k})$ in its real and imaginary parts $\sigma(\omega,\vec{k}) \equiv \sigma'(\omega,\vec{k}) + i\sigma''(\omega,\vec{k})$, where ω and $\vec{k}$ remain real-valued. Check that the shear viscosity coefficient can be related to the real part of $\sigma(\omega,\vec{k})$ according to

$$\eta = \lim_{\omega\to 0} n_0 m^2\omega^2 \lim_{\vec{k}\to\vec{0}} \frac{\sigma'(\omega,\vec{k})}{\vec{k}^2}.$$

Note that the order of the limits is important, and that you actually do not need to consider the limit of low frequencies to obtain the result. Yet writing both limits conveniently reminds you that hydrodynamics is a long-wavelength and low-frequency effective theory of a more microscopic description (as we shall see later in the lectures).

Comment: Equation (1)—or its equivalent ($\mathcal{E}$) in $(t,\vec{r})$-space—obviously express the *linear* response of the vorticity $\vec{\omega}$ to an excitation by an external force.

[2] Just for the sake of upsetting you I retain the traditional notations for the vorticity and the angular frequency!