Tutorial sheet 4

Discussion topic: Classical and quantum-mechanical Liouville operators

8. Linearised Navier–Stokes equation and shear viscosity

For a simple one-component fluid subject to an external force field (e.g. a gravity field), the Navier–Stokes equation takes the form

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

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 $\mathscr{n}$, $\vec{\mathsf{v}}$, 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 $\mathscr{n}_0$, $\vec{\mathsf{v}}_0=\vec{0}$, and $\mathcal{P}_0$ corresponding to a motionless fluid, for instance $\mathscr{n}(t,\vec{r})=\mathscr{n}_0+\delta\mathscr{n}(t,\vec{r})$ with $|\delta\mathscr{n}(t,\vec{r})|\ll\mathscr{n}_0$.

i. Linearise 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, $\mathscr{n}_0$, η, and $\vec{G}(t,\vec{r})\equiv\vec{\nabla}\times\vec{F}(t,\vec{r})$ — for the *vorticity* $\vec{\omega}(t,\vec{r})\equiv\vec{\nabla}\times\vec{\mathsf{v}}(t,\vec{r})$.[1] 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:[1]

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

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

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

where the "conductivity" $\sigma(\omega,\vec{k})$ depends, besides its variables, on the parameters m, $\mathscr{n}_0$, and η.

iii. Separate $\sigma(\omega,\vec{k})$ in its real and imaginary parts $\sigma(\omega,\vec{k})\equiv\sigma'(\omega,\vec{k})+\mathrm{i}\sigma''(\omega,\vec{k})$, 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

$$\eta=\lim_{\omega\to 0}\mathscr{n}_0m^2\omega^2\lim_{\vec{k}\to\vec{0}}\frac{\sigma'(\omega,\vec{k})}{\vec{k}^2}.$$

Note that the order of the limits is important, and that you actually do not need to consider the limit of low (angular) 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.

9. Liouville operator in classical mechanics

The lecture introduced the Liouville operator $\mathcal{L}$, acting on functions on the N-particle phase space Γ with canonical variables $(\{q_i\},\{p_i\})$. Let $\mathrm{d}^{6N}\mathcal{V}\propto\prod_i\mathrm{d}q_i\,\mathrm{d}p_i$ denote a uniform measure on Γ, as e.g. that used in the lecture.

i. Hermiticity of $\mathcal{L}$

Consider two functions $g(\{q_i\},\{p_i\})$, $h(\{q_i\},\{p_i\})$ which vanish sufficiently rapidly at infinity; let g^*, h^* denote the complex conjugate functions. Show that

$$\int_\Gamma g^*(\{q_i\},\{p_i\})\mathcal{L}h(\{q_i\},\{p_i\})\,\mathrm{d}^{6N}\mathcal{V}=\int_\Gamma(\mathcal{L}g)^*(\{q_i\},\{p_i\})h(\{q_i\},\{p_i\})\,\mathrm{d}^{6N}\mathcal{V}.$$

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

Recognizing in the integral over Γ of g^*h an inner product, which could be denoted as $\langle g, h\rangle$ — or with a bra-ket notation? —, the identity can be recast as $\langle g, \mathcal{L}h\rangle = \langle \mathcal{L}g, h\rangle$, which expresses the property that the Liouville operator is Hermitian[2] for this inner product.

ii. Unitarity of $\mathrm{e}^{\pm\mathrm{i}\mathcal{L}}$

Show that the operator $\mathrm{e}^{\mathrm{i}\mathcal{L}}$ acting on phase-space functions is unitary.

10. 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

$$\frac{\mathrm{d}\hat{O}(t)}{\mathrm{d}t} = \mathrm{i}\,\hat{\hat{\mathcal{L}}}\hat{O}(t).$$

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 the kets of $\mathscr{H}$ —, $\hat{O}^\dagger$ is the Hermitian conjugate[3] (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: write down the form of the Liouville operator! Only very short calculations are needed.

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

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

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

[2]... according to the physicists' denomination; mathematicians may prefer "self-adjoint".

[3]a.k.a. adjoint.