Microscopic Theory III: The Hydrodynamic Equations - part I

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1 Phenomenology

- The *hydrodynamic equations* specify how liquids and gases move collectively on meso and macro-scopic time and length scales.
  - They described transport of locally-defined mass density, fluid velocity, and energy in a liquid.
  - Form basis for simple aeronautics and fluid mechanics.
  - Are a basic part of our everyday experience with local temperatures, pressures etc.. that lead to motion, such as wind currents, sound and waves, and so on.
- Implicit in the hydrodynamic equations is the assumption of *local equilibrium:*
  - We can partition the full system into mesoscopically sized cells that are large compared to molecular length scales but small compared to the overall dimensions of the system.
  - Each cell is in a kind of equilibrium state, in which thermodynamic quantities can be defined locally (i.e. temperature, chemical potential). The normal thermodynamic relations between pressure, temperature and density are assumed to hold.
- The set of *hydrodynamic variables* consists of the locally-defined densities of mass (or particle number) $n(\mathbf{r},t)$, momentum $\mathbf{p}(\mathbf{r},t)$ and energy $e(\mathbf{r},t)$.
- The integrals over the entire system of each of these quantities gives a *time invariant* quantity since the variables are densities of conserved quantities of the dynamics.

$$\int_V d\mathbf{r}\, n(\mathbf{r},t) = N \qquad \int_V d\mathbf{r}\, \mathbf{p}(\mathbf{r},t) = \mathbf{P} \qquad \int_V d\mathbf{r}\, e(\mathbf{r},t) = E.$$

- It is useful to introduce a velocity field $\mathbf{v}(\mathbf{r},t)$ defined by the relation

$$\mathbf{p}(\mathbf{r},t) = mn(\mathbf{r},t)\mathbf{v}(\mathbf{r},t).$$

- Since the spatial integrals of these densities are conserved quantities, the time derivatives of the hydrodynamic variables are proportional to divergences of *currents*, leading to the *conservation equations*

$$\begin{aligned}
\dot{n}(\mathbf{r},t) &= -\frac{1}{m}\nabla\cdot\mathbf{p}(\mathbf{r},t) \\
\dot{\mathbf{p}}(\mathbf{r},t) &= -\nabla\cdot\sigma(\mathbf{r},t) \\
\dot{e}(\mathbf{r},t) &= -\nabla\cdot\mathbf{J}^{\mathbf{e}}(\mathbf{r},t),
\end{aligned}$$

  where σ is the momentum current or *stress tensor*, and $\mathbf{J}^{\mathbf{e}}$ is the energy current.

- These equations are supplemented by two *constitutive relations*, in which σ and $\mathbf{J^e}$ are expressed in terms of dissipative processes in the fluid.

- The changes in the local velocity field are related to local changes in the hydrostatic pressure $P_h(\mathbf{r},t)$ and a kind of fluid friction, or resistance to flow (viscosity), so:

$$\sigma^{\alpha\beta}(\mathbf{r},t) = \delta_{\alpha\beta}P_h(\mathbf{r},t) - \eta\left(\frac{\partial v_\alpha(\mathbf{r},t)}{\partial r_\beta} + \frac{\partial v_\beta(\mathbf{r},t)}{\partial r_\alpha}\right) + \delta_{\alpha\beta}\left(\frac{2}{3}\eta - \zeta\right)\nabla\cdot\mathbf{v}(\mathbf{r},t) = 0.$$

  - η is called the *shear viscosity*, and ζ is called the *bulk viscosity.* These are known as *transport coefficients.*

- We will assume that the local deviations of the hydrodynamic variables from their averages are small, so that we may linearize the equations with respect to deviations.

  - For example, $n(\mathbf{r},t) = n + \delta n(\mathbf{r},t)$, where $n = \rho$ is equilibrium bulk density.
  - Since $\mathbf{v}(\mathbf{r},t) = 0$ in an equilibrium liquid, we can linearize $\mathbf{p}(\mathbf{r},t)$ to get $\mathbf{p}(\mathbf{r},t) = mn\mathbf{v}(\mathbf{r},t)$.

- Substituting the constitutive relation for the stress tensor in the conservation equation for $\mathbf{p}(\mathbf{r},t)$ and linearizing gives

$$nm\dot{\mathbf{v}}(\mathbf{r},t) + \nabla P_h(\mathbf{r},t) - \eta\nabla^2\mathbf{v}(\mathbf{r},t) - \left(\frac{1}{3}\eta + \zeta\right)\nabla\nabla\cdot\mathbf{v}(\mathbf{r},t).$$

- Now looking at the equation for the energy flow, we use a second constitutive relation that describes energy changes as arising from enthalpy convection and temperature gradients:

$$\mathbf{J^e}(\mathbf{r},t) = h\mathbf{v}(\mathbf{r},t) - \lambda\nabla T(\mathbf{r},t),$$

  where $h = e + P_h$ is the enthalpy, and $T(\mathbf{r},t)$ is the local temperature.

  - The transport coefficient λ for temperature gradients is known as the *thermal conductivity.*

- Substition of this equation into the third of the conservation equations gives

$$\frac{\partial}{\partial t}\left[e(\mathbf{r},t) - \frac{e+P_h}{n}n(\mathbf{r},t)\right] - \lambda\nabla^2 T(\mathbf{r},t) = 0.$$

  - Note that it is useful to define the variable

$$\begin{aligned} Q(\mathbf{r},t) &= e(\mathbf{r},t) - \frac{e+P_h}{n}n(\mathbf{r},t) \quad \text{so that} \\ \dot{Q}(\mathbf{r},t) &= \lambda\nabla^2 T(\mathbf{r},t). \end{aligned}$$

  - $Q(\mathbf{r},t)$ can be interpreted as a *density* of heat energy since if the total number of particles is held fixed at N with $n = \rho = N/V$ then $dn = -ndV/V$ or $dV = -Vdn/n$ and

$$\begin{aligned} TdS &= dU + P_h dV = d(eV) + P_h dV \\ &= Vde + (e+P_h)dV = Vde - (e+P_h)Vdn/n \\ \frac{T}{V}dS &= dQ = de - \frac{e+P_h}{n}dn. \end{aligned}$$

- We now invoke the hypothesis of local equilibrium, in which the non-equilibrium, local thermodynamic quantities like the pressure $P_h(\mathbf{r},t)$ and heat density $Q(\mathbf{r},t)$ are *assumed* to depend on the independent variables, the local density $n(\mathbf{r},t)$ and temperature $T(\mathbf{r},t)$ just as they do in equilibrium.

- Expanding the deviations of the pressure and heat density to first order in deviations $\delta n(\mathbf{r},t) = n(\mathbf{r},t) - n$ and $\delta T(\mathbf{r},t) = T(\mathbf{r},t) - T$, we get

$$\begin{aligned}
\delta P_h(\mathbf{r},t) &= \left(\frac{\partial P_h}{\partial n}\right)_T \delta n(\mathbf{r},t) + \left(\frac{\partial P_h}{\partial T}\right)_n \delta T(\mathbf{r},t) \\
\delta Q(\mathbf{r},t) &= \frac{T}{V}\left[\left(\frac{\partial S}{\partial n}\right)_T \delta n(\mathbf{r},t) + \left(\frac{\partial S}{\partial T}\right)_n \delta T(\mathbf{r},t)\right] \\
&= nT\left(\frac{\partial S/N}{\partial n}\right)_T \delta n(\mathbf{r},t) + nc_V \delta T(\mathbf{r},t) \\
&= -\frac{T}{n}\left(\frac{\partial P_h}{\partial T}\right)_n \delta n(\mathbf{r},t) + nc_V \delta T(\mathbf{r},t).
\end{aligned}$$

- Inserting these relations in the equations of motion gives the *linearized hydrodynamic equations*,

$$\begin{aligned}
\frac{\partial \delta n(\mathbf{r},t)}{\partial t} + \nabla\cdot\mathbf{j}(\mathbf{r},t) &= 0 \\
\left(\frac{\partial}{\partial t} - a\nabla^2\right)\delta T(\mathbf{r},t) - \frac{T}{n^2 c_v}\left(\frac{\partial P_h}{\partial T}\right)_n \frac{\partial \delta n(\mathbf{r},t)}{\partial t} &= 0 \\
\left(\frac{\partial}{\partial t} - \frac{\eta}{mn}\nabla^2 - \frac{\eta/3+\zeta}{mn}\nabla\nabla\cdot\right)\mathbf{j}(\mathbf{r},t) + \left(\frac{\partial P_h}{\partial n}\right)_T \nabla\delta n(\mathbf{r},t) + \left(\frac{\partial P_h}{\partial T}\right)_n \nabla T(\mathbf{r},t) &= 0,
\end{aligned}$$

where $\mathbf{j}(\mathbf{r},t) = n\mathbf{v}(\mathbf{r},t)$ and $a = \lambda/nc_v$.

- These equations are solved by Fourier-Laplace transform methods:

$$\begin{aligned}
z\tilde{n}(\mathbf{k},z) - i\mathbf{k}\cdot\tilde{\mathbf{j}}(\mathbf{k},t) &= n(\mathbf{k}) \\
(z + ak^2)\tilde{T}(\mathbf{k},z) - \frac{T}{n^2 c_v}\left(\frac{\partial P_h}{\partial T}\right)_n i\mathbf{k}\cdot\tilde{\mathbf{j}}(\mathbf{k},z) &= T(\mathbf{k}) \\
\left(z + \frac{\eta}{mn}k^2 + \frac{\eta/3+\zeta}{mn}\mathbf{k}\mathbf{k}\cdot\right)\tilde{\mathbf{j}}(\mathbf{k},z) - \frac{i\mathbf{k}}{m}\left(\frac{\partial P_h}{\partial n}\right)_T \tilde{n}(\mathbf{k},z) - \frac{i\mathbf{k}}{m}\left(\frac{\partial P_h}{\partial T}\right)_n \tilde{T}(\mathbf{k},z) &= \mathbf{j}(\mathbf{k}).
\end{aligned}$$

- We can simplify the last equation somewhat by writing the current $\mathbf{j}(\mathbf{k})$ in longitudinal parts $\hat{\mathbf{k}}\cdot\mathbf{j}(\mathbf{k}) = \mathbf{j}^z(\mathbf{k})$ and transverse parts $\mathbf{j}^{x,y}(\mathbf{k})$, where we have chosen $\hat{\mathbf{k}}$ along the $\mathbf{z}$ direction.

$$\begin{aligned}
\left(z + bk^2\right)\tilde{\mathbf{j}}^z(\mathbf{k},z) - \frac{ik}{m}\left(\frac{\partial P_h}{\partial n}\right)_T \tilde{n}(\mathbf{k},z) - \frac{ik}{m}\left(\frac{\partial P_h}{\partial T}\right)_n \tilde{T}(\mathbf{k},z) &= \mathbf{j}^z(\mathbf{k}) \\
(z + \nu k^2)\mathbf{j}^\alpha(\mathbf{k},z) &= \mathbf{j}^\alpha(\mathbf{k}) \quad \alpha = x,y,
\end{aligned}$$

where

$$b = \frac{4\eta/3+\zeta}{mn} \qquad \nu = \frac{\eta}{mn}.$$

- Defining the vectors:

$$\tilde{A}(\mathbf{k},z) = \{\tilde{n}(\mathbf{k},z), \tilde{T}(\mathbf{k},z), \tilde{\mathbf{j}}^z(\mathbf{k},z), \tilde{\mathbf{j}}^x(\mathbf{k},z), \tilde{\mathbf{j}}^y(\mathbf{k},z)\} \qquad A(\mathbf{k}) = \{n(\mathbf{k}), T(\mathbf{k}), \mathbf{j}^z(\mathbf{k}), \mathbf{j}^x(\mathbf{k}), \mathbf{j}^y(\mathbf{k})\},$$

these equation can be written in compact matrix form:

$$\begin{aligned} [z\mathbf{I} - \mathbf{M}(\mathbf{k})] \cdot \tilde{A}(\mathbf{k},z) &= A(\mathbf{k}) \\ \tilde{A}(\mathbf{k},z) &= [zI - \mathbf{M}(\mathbf{k})]^{-1} \cdot A(\mathbf{k}), \end{aligned}$$

where we have defined the *hydrodynamic matrix* $\mathbf{M}(\mathbf{k},z)$ to be

$$\mathbf{M}(\mathbf{k}) = \begin{pmatrix} 0 & 0 & ik & 0 & 0 \\ 0 & -ak^2 & \frac{ikT}{n^2 c_v}\left(\frac{\partial P_h}{\partial T}\right)_n & 0 & 0 \\ \frac{ik}{m}\left(\frac{\partial P_h}{\partial n}\right)_T & \frac{ik}{m}\left(\frac{\partial P_h}{\partial T}\right)_n & -bk^2 & 0 & 0 \\ 0 & 0 & 0 & -\nu k^2 & 0 \\ 0 & 0 & 0 & 0 & -\nu k^2 \end{pmatrix}.$$

- Note that the transverse ("shear") velocity modes are decoupled from all other modes and can be solved exactly to get

$$\begin{aligned} \tilde{\mathbf{j}}^\alpha(\mathbf{k},z) &= \frac{\mathbf{j}^\alpha(\mathbf{k})}{z + \nu k^2} \quad \text{so} \\ \mathbf{j}^\alpha(\mathbf{k},t) &= e^{-\nu k^2 t}\mathbf{j}^\alpha(\mathbf{k}). \end{aligned}$$

  - Exponential decay of initial non-equilibrium flow $m\mathbf{v}^\alpha(\mathbf{k})$, with life-time $\tau_v = 1/(\nu k^2)$.
  - Long-wavelength modes with small k decay very slowly on molecular time scales since $\nu k^2 t_m << 1$.
  - Relaxation times that scale as k^{-2} are typical of hydrodynamic modes.

- The evolution of the 3 other modes can be approximately calculated using the minor formula:

$$[z\mathbf{I} - \mathbf{M}(\mathbf{k},z)]^{-1}_{\alpha\beta} = \frac{(-1)^{\alpha+\beta}\mathcal{M}_{\beta\alpha}}{\det|z\mathbf{I} - \mathbf{M}(\mathbf{k},z)|},$$

where $\mathcal{M}_{ij}$ is the determinant of the minor matrix formed by crossing out the *ith* row and *jth* column of the full matrix $\mathbf{M}(\mathbf{k},z)$.

- The determinant gives a cubic equation in z. The roots of this are relevant for Laplace inversion since one can write the expression above as

$$\begin{aligned} \frac{(-1)^{\alpha+\beta}\mathcal{M}_{\beta\alpha}}{\det|z\mathbf{I} - \mathbf{M}(\mathbf{k},z)|} &= \frac{f(\mathbf{k},z)}{(z-z_1)(z-z_2)(z-z_3)} \\ &= \frac{1}{z-z_1}\frac{f(\mathbf{k},z_1)}{(z_1-z_2)(z_1-z_3)} + \frac{1}{z-z_2}\frac{f(\mathbf{k},z_2)}{(z_2-z_1)(z_2-z_3)} + \frac{1}{z-z_3}\frac{f(\mathbf{k},z_3)}{(z_3-z_2)(z_3-z_1)} \\ &= \frac{a_1}{z-z_1} + \frac{a_2}{z-z_2} + \frac{a_3}{z-z_3} \end{aligned}$$

where $f(\mathbf{k},z)$ is a polynomial of lower degree than the denominator.

- This can be inverted to give the sum of three exponentials:

$$\mathcal{L}^{-1}\frac{(-1)^{\alpha+\beta}\mathcal{M}_{\beta\alpha}}{\det|z\mathbf{I}-\mathbf{M}(\mathbf{k},z)|} \quad = \quad a_1 e^{z_1 t} + a_2 e^{z_2 t} + a_3 e^{z_3 t}.$$

- The roots z_i can be solved by expanding $z_i = z_i^{(0)} + z_i^{(1)}k + z_i^{(2)}k^2 + \ldots$ in powers of k and solving for the coefficients $z_i^{(j)}$ order by order (homework).
  - One obtains the roots (homework)

$$z_0 = -\Gamma_T k^2 \qquad z_\pm = \pm i c_0 k - \Gamma_s k^2$$

    with

$$\Gamma_T = \frac{a}{\gamma} = \frac{\lambda}{nc_p} \qquad \Gamma_s = \frac{1}{2}\left[a(\gamma-1)/\gamma + b\right]$$

    where $\gamma = c_p/c_v$.

- Using this approach, it can be shown that the Fourier transform of the number density is given by

$$n(\mathbf{k},t) \quad = \quad n(\mathbf{k})\left[\frac{1}{\gamma}\cos(c_0 kt)\, e^{-\Gamma_s k^2 t} + \frac{\gamma-1}{\gamma}e^{-\Gamma_T k^2 t}\right].$$

  where $c_0 = \frac{\gamma}{m}\left(\frac{\partial P}{\partial n}\right)_T$ is the "adiabatic sound speed".
  - The equation above can be viewed as arising from a propagating sound mode (with frequency $c_0 k$) and to thermal diffusion.