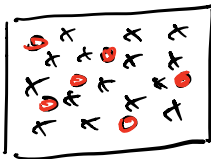


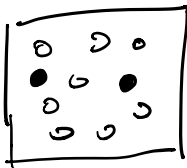
## Diffusion and heat conduction

We continue with the calculation of transport coefficients and now consider the response of a system to temperature and density gradients

Since in single component systems, temperature or density gradients lead to macroscopic motions described by hydrodynamics in the limit  $\lambda_{\text{MFP}} \ll \ell$  we will consider one of the two following situations



Lorentz gas: Collection of light particles interacting with heavy particles acting as static scattering centers



Self-diffusion  
or dilute tracer:

Evolution of e.g. radial velocity involved atoms in dilute gas of atoms

Clearly in both cases the interaction with other particles allows for momentum exchange

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We consider that local equilibrium conditions  $T(t, \vec{r})$  and  $\mu(t, \vec{r})$  are determined externally e.g. by controlling the temperature of the background medium and redressing excitation of atoms such that

$$T(t, \vec{r}) = T(\vec{r}) \quad \mu(t, \vec{r}) = \mu(\vec{r})$$

are both time independent, and the local equilibrium solution for our system takes the form

$$O(U_n^0) \quad \psi^{(0)}(t, \vec{r}; \vec{p}) = \psi^{(0)}(\vec{r}; \vec{p}) = e^{\frac{\mu(\vec{r})}{k_B T(\vec{r})}} e^{-\frac{\vec{p}^2}{2mk_B T(\vec{r})}}$$

where instead of our usual velocity means of  $v(\vec{r})$ , we have employed the chemical potential  $\mu(\vec{r})$  to make contact with operators  $(\vec{\nabla}(\frac{1}{T}), \vec{\nabla}(-\frac{\mu}{T}))$  that appear in macroscopic description

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Now if we look at the non-equilibrium corrections  $f^{(1)}$  due to temperature and chemical potential gradients, we expand

$$f = f^{(0)} + f^{(1)} + \dots$$

and find that in the limit  $h\nu \ll kT$ , the Hilbert expansion yields

$$O(h\nu): \quad \frac{\vec{p}}{m} \vec{\nabla}_r f^{(0)}(\vec{r}, \vec{p}) = \delta C [f^{(0)}, f^{(1)}]^{RTA} = - \frac{f^{(1)}(\vec{r}, \vec{p})}{\tau_R}$$

Now evaluating the derivatives of  $f^{(0)}(\vec{r}, \vec{p})$

$$\vec{\nabla}_r f^{(0)}(\vec{r}, \vec{p}) = - \frac{1}{k_B} \left[ \frac{\vec{p}^2}{2m} \vec{\nabla}_r \left( \frac{1}{T(\vec{r})} \right) + \vec{\nabla}_r \left( - \frac{\mu(\vec{r})}{T(\vec{r})} \right) \right] f^{(0)}(\vec{r}, \vec{p})$$

we have a stationary solution for  $f^{(1)}$

$$f^{(1)}(\vec{r}, \vec{p}) = \frac{\tau_R}{m k_B} \vec{p} \left[ \frac{\vec{p}^2}{2m} \vec{\nabla}_r \left( \frac{1}{T(\vec{r})} \right) + \vec{\nabla}_r \left( - \frac{\mu(\vec{r})}{T(\vec{r})} \right) \right] f^{(0)}(\vec{r}, \vec{p})$$

i.e. one term proportional to each affinity

$$\vec{\nabla}_r \left( \frac{1}{T(\vec{r})} \right), \quad \vec{\nabla}_r \left( - \frac{\mu(\vec{r})}{T(\vec{r})} \right)$$

Now we can compute the associated  
 particle and energy fluxes

$$\mathcal{J}_N^i = \int_{\vec{p}} \frac{p^i}{m} (f^{(0)} + f^{(1)}) \stackrel{f^{(0)} \text{ isotropic}}{=} \int_{\vec{p}} \frac{p^i}{m} f^{(1)}$$

$$\mathcal{J}_E^i = \int_{\vec{p}} \frac{p^i}{m} \frac{\vec{p}^2}{2m} (f^{(0)} + f^{(1)}) \stackrel{f^{(0)} \text{ isotropic}}{=} \int_{\vec{p}} \frac{p^i}{m} \frac{\vec{p}^2}{2m} f^{(1)}$$

Now specializing at the expressions, we get  
 for  $\bar{\epsilon}_R = \text{const}$

$$\mathcal{J}_N^i = \frac{\bar{\epsilon}_R}{m k_B} \int_{\vec{p}} \frac{p^i p_j}{m} \left[ \frac{\vec{p}^2}{2m} \frac{1}{\partial f_j} \left( \frac{1}{T(\vec{r})} \right) + \frac{d}{df_j} \left( -\frac{\mu(\vec{r})}{T(\vec{r})} \right) \right] f^{(0)}(\vec{r}, \vec{p})$$

$$\mathcal{J}_E^i = \frac{\bar{\epsilon}_R}{m k_B} \int_{\vec{p}} \frac{p^i p_j}{m} \frac{\vec{p}^2}{2m} \left[ \frac{\vec{p}^2}{2m} \frac{1}{\partial f_j} \left( \frac{1}{T(\vec{r})} \right) + \frac{d}{df_j} \left( -\frac{\mu(\vec{r})}{T(\vec{r})} \right) \right] f^{(0)}(\vec{r}, \vec{p})$$

where again due to the isotropy of  
 $f^{(0)}$  the response is isotropic in the  
 sense that

$$\int_{\vec{p}} p_i p_j h(\vec{p}^2) \psi^{(0)}(\vec{r}, \vec{p}) = \frac{1}{3} \delta^{ij} \int_{\vec{p}} p^2 h(\vec{p}^2) \psi^{(0)}(\vec{r}, \vec{p})$$

such that the constitutive relations take the form

$$\underline{\vec{J}}_N = \frac{2\bar{c}R}{3\pi h_3} \int_{\vec{p}} \frac{\vec{p}}{2m} \left[ \frac{\vec{p}}{2m} \underline{\vec{\nabla}}_r \left( \frac{1}{T(r)} \right) + \underline{\vec{\nabla}}_r \left( -\frac{M(r)}{T(r)} \right) \right] \psi^{(0)}(\vec{r}, \vec{p})$$

$$\underline{\vec{J}}_e = \frac{2\bar{c}R}{3\pi h_3} \int_{\vec{p}} \left( \frac{\vec{p}}{2m} \right)^2 \left[ \frac{\vec{p}}{2m} \underline{\vec{\nabla}}_r \left( \frac{1}{T(r)} \right) + \underline{\vec{\nabla}}_r \left( -\frac{M(r)}{T(r)} \right) \right] \psi^{(0)}(\vec{r}, \vec{p})$$

which reflects Curie principle in the sense that if no current is generated from a linear constitutive relation

$$\vec{J}_N^\alpha = L_{Nn}^{\alpha\beta} \frac{\partial Y_n}{\partial r^\beta} \text{ we have } L_{Nk}^{\alpha\beta} = \delta^{\alpha\beta} L_{Nn}$$

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By comparing the microscopic expressions for  $\vec{J}_N$  and  $\vec{J}_E$  with the explicit form of the linear constitutive relations

$$\vec{J}_N = L_{NN} \vec{v}\left(-\frac{\mu}{T}\right) + L_{NE} \vec{v}\left(\frac{1}{T}\right)$$

$$\vec{J}_E = L_{EN} \vec{v}\left(-\frac{\mu}{T}\right) + L_{EE} \vec{v}\left(\frac{1}{T}\right)$$

we can then read off the coefficients  $L_{NN}$ ,  $L_{NE}$ ,  $L_{EN}$ ,  $L_{EE}$

Evaluating the integrals as

$$\int_{\vec{p}} \frac{\vec{p}}{2m} f^{(0)} = e = \frac{3}{2} n k_B T$$

$$\int_{\vec{p}} \left(\frac{\vec{p}}{2m}\right)^2 f^{(0)} = \frac{5}{2} k_B T e$$

$$\int_{\vec{p}} \left(\frac{\vec{p}}{2m}\right)^3 f^{(0)} = \frac{35}{4} (k_B T)^2 e$$

this becomes a matter of simple algebra yielding

$$L_{NN} = \frac{n\bar{c}RT}{m}$$

$$L_{NE} = \frac{5}{2} \frac{n\bar{c}RT}{m} k_B T$$

$$L_{EN} = \frac{5}{2} \frac{n\bar{c}RT}{m} k_B T$$

$$L_{EE} = \frac{35}{4} \frac{n\bar{c}RT}{m} (k_B T)^2$$

when we see that a larger relaxation time  $\bar{c}_R$  leads to stronger diffusion and heat conduction

We also explicitly verify Onsager relations such that in this case  $L_{NE} = L_{EN}$