Statistical Mechanics - Homework 10

M. Ross Tagaras (Dated: December 2, 2020)

PROBLEM 1

Part (a)

By the master equation,

$$\frac{\partial}{\partial t} \sum_{i} w_i = \sum_{i,j} P_{ij}(w_j - w_i)$$

This quantity vanishes by symmetry.

Part (b)

The entropy is

$$S = -\text{Tr}(\rho \ln \rho) = -\sum_{i} w_{i} \ln w_{i}$$

The derivative of entropy is

$$\frac{dS}{dt} = -\sum_{i} \frac{dw_i}{dt} \ln w_i - \sum_{i} \frac{w_i}{w_i} \frac{\partial w_i}{\partial t} = \sum_{i,j} P_{ij}(w_i - w_j) \left(\ln w_i + 1\right)$$

Using the symmetry of P_{ij} :

$$\frac{dS}{dt} = \frac{1}{2} \sum_{i,j} (P_{ij} + P_{ji})(w_i - w_j) (\ln w_i + 1) = \frac{1}{2} \sum_{i,j} P_{ij} \left[(w_i - w_j)(\ln w_i + 1) - (w_i - w_j)(\ln w_j + 1) \right]$$

$$= \frac{1}{2} \sum_{i,j} P_{ij} (w_i - w_j) (\ln w_i - \ln w_j)$$

If $w_i > w_j$, $\ln w_i > \ln w_j$, so each term in the sum is positive. If $w_i < w_j$, then $\ln w_i < \ln w_j$, and the negative signs combine, again resulting in a sum of positive terms. Therefore, S is monotonically increasing.

Part (c)

The master equation gives

$$\frac{\partial w_1}{\partial t} = p(w_2 - w_1) \qquad \frac{\partial w_2}{\partial t} = p(w_1 - w_2) = -\frac{\partial w_1}{\partial t}$$

With the initial conditions $w_1(0) = 1$, $w_2(0) = 0$, we find

DSolve[{w1'[t] == p (w2[t] - w1[t]), w2'[t] == p (w1[t] - w2[t]), w1[0] == 1, w2[0] == 0}, {w1, w2}, t] Out[100] = $\left\{ \left\{ w1 \rightarrow \mathsf{Function} \left[\left\{ t \right\}, \, \frac{1}{2} \, e^{-2 \, p \, t} \, \left(1 + e^{2 \, p \, t} \right) \, \right], \, w2 \rightarrow \mathsf{Function} \left[\left\{ t \right\}, \, \frac{1}{2} \, e^{-2 \, p \, t} \, \left(-1 + e^{2 \, p \, t} \right) \, \right] \right\} \right\}$

so the time dependent w_i are

$$w_1(t) = \frac{1}{2} \left(1 + e^{-2pt} \right)$$
 $w_2(t) = \frac{1}{2} \left(1 - e^{-2pt} \right)$

PROBLEM 2

Adding a factor of $e^{i\omega t}$ for time dependence and calculating \tilde{w} gives

$$-\frac{\tilde{w}}{\tau} = \left(\frac{\partial w}{\partial t} + q\vec{E} \cdot \frac{\vec{p}}{m} \frac{\partial w_0}{\partial \varepsilon}\right) \implies \tilde{w} = -\tau i \omega \tilde{w} - \tau \frac{q}{m} \vec{E} \cdot \vec{p} \frac{\partial w_0}{\partial \varepsilon}$$

so we find

$$\tilde{w} = -\frac{\tau}{1-i\omega\tau} \frac{q}{m} \vec{E} \cdot \vec{p} \frac{\partial w_0}{\partial \varepsilon}$$

This is the same result for \tilde{w} that we used in the time-independent case, except for the overall factor of $\frac{1}{1-i\omega\tau}$, which is independent of p. Therefore, the integration over \vec{p} in the definition of \vec{j} is the same, and we find

$$\sigma(\omega) = \frac{\sigma(0)}{1 - i\omega\tau}$$

In Joule heating, the power density is

$$P/V = \vec{j} \cdot E = |\sigma| E^2 = \left| \frac{\sigma(0)}{1 - i\omega\tau} \right| E^2 = \frac{\sigma(0)E^2}{\sqrt{1 + \omega^2\tau^2}}$$

This should be real-valued, so I took the absolute value. When $\omega \tau \gg 1$, this is approximately

$$P/V \approx \frac{\sigma(0)E^2}{\omega \tau}$$

PROBLEM 3

Part (a)

The electric conductivity is found from the current:

$$\vec{j} = q \int d^3p \ \vec{v}\tilde{w} = \sigma \vec{E}$$

The Liouville equation with the RTA gives (assuming spatial uniformity)

$$\tilde{w} = -\tau q E_i \frac{\partial w_0}{\partial p_i}$$

Then, we have

$$\sigma E_i = -\tau q \int d^3 p \frac{p_i}{m} \left[q E_j \frac{\partial w_0}{\partial p_j} \right]$$

In equilibrium, w_0 is given by

$$w_0 = \frac{g}{(2\pi\hbar)^3} \left\langle N(\varepsilon) \right\rangle = \frac{g}{(2\pi\hbar)^3} e^{-(\varepsilon - \mu)/T} = \frac{g}{(2\pi\hbar)^3} e^{\frac{\mu}{T} - \frac{p^2}{2mT}}$$

so our expression for σ reduces to

$$\sigma E_{i} = \frac{\tau q^{2} g E_{j}}{m^{2} (2\pi \hbar)^{3} T} e^{\mu/T} \int d^{3} p \ p_{i} p_{j} e^{-\frac{p^{2}}{2mT}}$$

Integrating (for example, the i = 1 component) gives

Integrate [Integrate [Integrate [p1 (E1 p1 + E2 p2 + E3 p3) $e^{\frac{-1}{2 m T} \left(p1^2 + p2^2 + p3^2\right)}, \{p1, -\infty, \infty\}], \{p2, -\infty, \infty\}], \{p3, -\infty, \infty\}]$ Out[105]=
ConditionalExpression $\left[2\sqrt{2} \text{ E1 m}^3 \pi^{3/2} \sqrt{\frac{1}{m T}} T^3, \text{Re}\left[\frac{1}{m T}\right] > 0\right]$

After simplifying, we find

$$\sigma E_i = \frac{\tau q^2 g \sqrt{m} T^2}{(2\pi \hbar^2)^{3/2}} e^{\mu/T} E_i \implies \sigma = \frac{\tau q^2 g \sqrt{m} T^2}{(2\pi \hbar^2)^{3/2}} e^{\mu/T}$$

Part (b)

The thermal conductivity is defined by the heat flow density:

$$h_i = \int d^3 p(\varepsilon - \mu) v_i \tilde{w} = -\kappa \frac{\partial T}{\partial x^i}$$

Likharev equation (6.55) gives an expression for \tilde{w} :

$$\tilde{w} = \tau \frac{\varepsilon - \mu}{T} v_i \frac{\partial T}{\partial x^i} \frac{\partial w}{\partial \varepsilon} = \frac{g\tau}{T^2 (2\pi\hbar)^3} e^{\mu/T} v_i \frac{\partial T}{\partial x^i} \left[\mu - \frac{p^2}{2m} \right] e^{-\frac{p^2}{2mT}}$$

This gives

$$\kappa \frac{\partial T}{\partial x^i} = \frac{g\tau}{T^2 m^2 (2\pi\hbar)^3} e^{\mu/T} \int d^3p \ p_i p_j \frac{\partial T}{\partial x^j} \left(\frac{p^2}{2m} - \mu\right)^2 e^{-\frac{p^2}{2mT}}$$

Integrating as before, we find

Integrate [Integrate [Integrate [$\frac{-\tau g}{m^2 T^2 (2\pi h)^3} e^{\frac{\mu}{t}} p1 (p1 T1 + p2 T2 + p3 T3) \left(\frac{p1^2 + p2^2 + p3^2}{2 m} - \mu \right)^2 e^{\frac{-1}{2 mT} \left(p1^2 + p2^2 + p3^2\right)}, \{p1, -\omega, \omega\}], \{p2, -\omega, \omega\}], \{p3, -\omega, \omega\}]$ Conditional Expression [$-\frac{e^{\frac{\mu}{t}} g T1 \left(35 T^2 - 20 T \mu + 4 \mu^2\right) \tau}{8 \sqrt{2} h^3 \pi^{3/2} \sqrt{\frac{1}{mT}}}$, Re[$\frac{1}{mT}$] > 0]

which results in

$$\kappa = \frac{g\tau e^{\mu/T}\sqrt{mT}\left(4\mu^2 + 35T^2 - 20\mu T\right)}{8\sqrt{2}\pi^{3/2}\hbar^3}$$

Part (c)