5.72 Problem set #6 J. Cao

(The problems can be solved by following the lecture notes.)

I. The self-intermediate scattering function $F_s(k,t) = \langle e^{-ik[z(t)-z(0)]} \rangle$ can be expressed in even moments

$$C_{2n} = (-1)^n F_s^{(0,2n)}(k,0).$$

1) Show $C_0 = 1$, $C_2 = \omega_0^2$, and $C_4 = 3\omega_0^4 + \omega_0^2\Omega_0^2$, where $\omega_0^2 = k^2 \frac{k_B T}{M}$ and Ω_0 is the Einstein frequency.
2) For free particles, show $F_s(k,t) = \exp\left[-\frac{1}{2}\omega_0^2 t^2\right]$.
3) Under what conditions for k can we ignore molecular collisions?

II. Calculate the velocity auto-correlation function $C(t) = \langle v(t)v(0) \rangle$ from the generalized Langevin equation.

1) Show C satisfies $\dot{C}(t) + \int_0^t \gamma(t-\tau)C(\tau)d\tau = 0$.
2) Show $\gamma(0) = \Omega_0^2$.
3) Derive the Laplace-transformed solution $\hat{C}(s) = \frac{v_0^2}{s+\hat{\gamma}(s)}$ and show $\hat{\gamma}(0) = (D\beta M)^{-1}$.
4) Solve $C(t)$ for the exponential decay memory kernel $\gamma(t) = \gamma(0)e^{-t/\tau}$.

III. The transverse current correlation function is defined as

$$C(k,t) = \frac{1}{N}\langle J_x(k,t) | J_x(k,0) \rangle.$$

1) Use GLE to derive $\dot{C}(t) + k^2 \int_0^t \nu(k,t-\tau)C(\tau)d\tau = 0$.
2) Show the two-limiting cases of $\nu(k,t)$:

$$\nu(k,0) = c_t^2(k),$$

where $c_t(k)$ is the transverse speed of sound, and

$$\int_0^\infty \nu(k,\tau)d\tau = \frac{\eta}{\rho m}.$$

3) Solve for $C(k,t)$ with the memory kernel $\nu(k,t) = \nu(k,0)e^{-t/\tau}$.

IV. *The transverse and longitudinal current correlation functions are

$$C_T(k,t) = \frac{1}{N}\langle J_T(k,t) | J_T(k,0) \rangle$$

and

$$C_L(k,t) = \frac{1}{N}\langle J_L(k,t)|J_L(k,0)\rangle,$$

respectively.

1) Show

$$C_T(k,t) = v_0^2\left(1 - \frac{\omega_T^2}{2}t^2 + \cdots\right),$$

where $\omega_T^2 = \omega_0^2 + \Omega_0^2 - \Omega_t^2$ and $\Omega_t^2 = \frac{\rho}{M}\int g(r)\partial_x^2\Phi e^{ikz}d\vec{r}$.

2) Show

$$C_L(k,t) = v_0^2\left(1 - \frac{\omega_L^2}{2}t^2 + \cdots\right),$$

where $\omega_L^2 = 3\omega_0^2 + \Omega_0^2 - \Omega_L^2$, $\Omega_L^2 = \frac{\rho}{M}\int g(r)\partial_z^2\Phi e^{ikz}d\vec{r}$.

V. *Correlation function moments

1) Show that the first three moments for the memory function are $k_0 = \frac{C_2}{C_0}$, $k_2 = \left(C_4 - \frac{C_2^2}{C_0}\right)\frac{1}{C_0}$, and $k_4 = \left(C_4 - \frac{2\,C_2C_4}{C_0} + \frac{C_2^3}{C_0^3}\right)\frac{1}{C_0}$, where $C_{2n} = \left\langle A^{(n)}\middle|A^{(n)}\right\rangle$ are the moments for the correlation functions.

2) Use the moments for $k(t)$ to verify the accuracy of GLE

$$\dot{C}(t) + \int_0^t k(t-\tau)C(\tau)d\tau = 0$$

to $o(t^6)$.

VI. *Define the projection operator as $\sum_\alpha P_\alpha$ with P_α being the projection operator for $A_\alpha = \rho_s(k)J_\alpha^x(k)$. Derive the mode-coupling expression

$$C(t) = \langle V(t)V(0)\rangle = \frac{v_0^2}{12\rho[\pi(D+\nu)t]^{3/2}}.$$