Problem set # 3 for 5.72 (spring 2012) Cao

I. A Gaussian variable with $\langle x \rangle = 0$ and $\langle x^2 \rangle = g$ is described by the probability function

$$p(x) = \frac{1}{\sqrt{2\pi g}} e^{-\frac{x^2}{2g}}.$$

1) Calculate $I(z) = \int_{-\infty}^{\infty} p(x) e^{zx} dx$.
2) Show that $\langle x^{2n} \rangle = \frac{(2n)!}{2^n n!} g^n$.

II. A Brownian particle in the potential of a constant force F follows

$$m\dot{v} + \zeta v = F + f,$$

where f is white noise with $\langle f \rangle = 0$ and $\langle f(t) f(0) \rangle = g\delta(t)$.

1) Given the initial velocity v_0, show that

$$\langle v(t) \rangle = v_0 e^{-\gamma t} + \frac{F}{\zeta}(1 - e^{-\gamma t}),$$

where $\gamma = \frac{\zeta}{m}$.

2) From the stationary condition $\langle v^2 \rangle - \langle v \rangle^2 = \frac{k_B T}{m}$, prove $g = 2k_B T\zeta$.
3) Show that $C(t) = \langle v(t) v(0) \rangle = \left(\frac{F}{\zeta}\right)^2 + \frac{k_B T}{m} e^{-\gamma t}$.
4) Calculate the mean square displacement $\langle |x(t) - x(0)|^2 \rangle$.

III. *Chandraskhar's theorem (see McQuarrie). White noise f is a Gaussian variable with $\langle f \rangle = 0$ and $\langle f(t_1) f(t_2) \rangle = g\delta(t_1 - t_2)$. If $A = \int_0^t a(\tau) f(\tau) d\tau$, the probability distribution of A is

$$P(A) = \frac{1}{\sqrt{2\pi\alpha(t)}} \exp\left[-\frac{A^2}{2\alpha(t)}\right],$$

where $\alpha(t) = g \int_0^t a^2(\tau) d\tau$.

1) Prove the theorem, i.e., Eq. (1)
2) For a Brownian particle, given the initial velocity v_0, find the probability distribution of v at time t, $p(v_0, v, t)$.
3) Show that the probability distribution of the displacement at time t, subject to the initial condition $x(0) = x_0$ and $v(0) = v_0$, is

$$p(x_0, v_0; x, t) = \frac{1}{\sqrt{2\pi\alpha(t)}} \exp\left[-\frac{\left[x - x_0 - \frac{v_0}{\gamma}(1 - e^{-\gamma t})\right]^2}{2\alpha(t)}\right],$$

with $\alpha(t) = \frac{D}{\gamma}(2\gamma t - 3 - e^{-2\gamma t} + 4e^{-\gamma t})$.

IV. Zwanzig (J. Stat. Phys. 9, p 215, 1973) proposed the system-bath Hamiltonian

$$H = \frac{p^2}{2M} + V(q) + \sum_i \frac{1}{2} m_i \dot{x}_i^2 + \frac{1}{2} m_i \omega_i^2 \left(x_i - \frac{c_i}{m_i \omega_i^2} q \right)^2$$

where $\{m_i, \omega_i, x_i\}$ define a set of bath harmonic modes.

1) Show that the reduced equation of motion for q is

$$M\ddot{q} + \int_0^t \zeta(t-\tau)\dot{q}(\tau)d\tau + \nabla V(q) = f(t).$$

2) Write the explicit form for $f(t)$ as a function of $x_i(0)$ and $\dot{x}_i(0)$.
3) Use the equilibrium conditions for $x_i(0)$ and $\dot{x}_i(0)$ to prove

$$\zeta(t) = \beta\langle f(t)f(0)\rangle = \sum_i \frac{c_i^2}{m_i \omega_i^2} \cos(\omega_i t).$$