DETERMINING NOISE FROM DETERMINSTIC FORCES

Consider the following deterministic equations

$$dX_\alpha = V_\alpha dt \tag{1}$$

and

$$dV_\alpha = -U_\alpha dt - \nabla\phi(\mathbf{X})dt. \tag{2}$$

We assume that U_α are generated by hydrodynamic interactions which do not however affect the equilibrium Gibbs Boltzmann distribution which is

$$P_{eq}(\mathbf{X},\mathbf{V}) = \frac{1}{\bar{Z}}\exp(-\frac{\beta\mathbf{V}^2}{2} - \beta\phi(\mathbf{X})) \tag{3}$$

The Fokker Planck equation at finite temperature which introduces white noise and possibly temperature dependent drifts is $\phi(\mathbf{X})$ is

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial V_\alpha}\left[T\gamma_{\alpha\beta}\frac{\partial P}{\partial V_\beta} + U_\alpha P + \frac{\partial\phi}{\partial X_\alpha}P\right] - \frac{\partial}{\partial X_\alpha}V_\alpha P \tag{4}$$

We obtain the GB distribution for the steady state if

$$U_\alpha = \gamma_{\alpha\beta}V_\beta \tag{5}$$

We have for small velocities that

$$U_\alpha = \lambda_{\alpha\beta}(\mathbf{X})V_\beta + \Lambda_{\alpha\beta\gamma}V_\beta V_\gamma, \tag{6}$$

and so we find

$$\gamma_{\alpha\beta}V_\beta = \lambda_{\alpha\beta}(\mathbf{X})V_\beta + \Lambda_{\alpha\beta\gamma}(\mathbf{X})V_\beta V_\gamma \tag{7}$$

Written this way the term $\lambda_{\alpha\beta}(\mathbf{X})$ is just the friction tensor in the absence of any elastic effects. We can thus write

$$\gamma_{\alpha\beta} = \lambda_{\alpha\beta} + \gamma_{2\alpha\beta} \tag{8}$$

and we write

$$\gamma_{2\alpha\beta} = \Gamma_{\alpha\beta\gamma}V_\gamma \tag{9}$$

and

$$\Gamma_{\alpha\beta\gamma}V_\beta V_\gamma = \Lambda_{\alpha\beta\gamma}V_\beta V_\gamma, \tag{10}$$

where we without loss of generality take $\Lambda_{\alpha\beta\gamma} = \Lambda_{\alpha\gamma\beta}$ This then gives

$$\Gamma_{\alpha\beta\gamma} + \Gamma_{\alpha\gamma\beta} = 2\Lambda_{\alpha\beta\gamma}. \tag{11}$$

We have to solve this system with the constraint that $\Gamma_{\alpha\beta\gamma}V_\gamma = \Gamma_{\beta\alpha\gamma}V_\gamma$. In Thomas' problem we have

$$U_z = \xi\frac{V_z}{Z^{\frac{3}{2}}} + \frac{21\kappa\xi}{4}\frac{V_z^2}{Z^{\frac{9}{2}}} - \frac{\kappa\xi}{4}\frac{V_x^2}{Z^{\frac{7}{2}}} \tag{12}$$

and

$$U_x = 2\xi\epsilon\frac{V_x}{3Z^{\frac{1}{2}}} + \frac{19\kappa\xi\epsilon}{24}\frac{V_zV_x}{Z^{\frac{7}{2}}} \tag{13}$$

Form this we find that

$$\begin{aligned}\sum_{\alpha\beta}\Lambda_{z\alpha\beta}V_\alpha V_\beta &= \frac{21\kappa\xi}{4}\frac{V_z^2}{Z^{\frac{9}{2}}} - \frac{\kappa\xi}{4}\frac{V_x^2}{Z^{\frac{7}{2}}}\\ \sum_{\alpha\beta}\Lambda_{x\alpha\beta}V_\alpha V_\beta &= \frac{19\kappa\xi\epsilon}{24}\frac{V_zV_x}{Z^{\frac{7}{2}}}\end{aligned} \tag{14}$$

This gives the set of equations

$$\Gamma_{zzz} = \frac{21\kappa\xi}{4Z^{\frac{9}{2}}} \tag{15}$$

$$\Gamma_{zxx} = -\frac{\kappa\xi}{4Z^{\frac{7}{2}}} \tag{16}$$

$$\Gamma_{zxz} + \Gamma_{zzx} = 0 \tag{17}$$

$$\Gamma_{xzz} = 0 \tag{18}$$

$$\Gamma_{xxx} = 0 \tag{19}$$

$$\Gamma_{xxz} + \Gamma_{xzx} = \frac{19\kappa\xi\epsilon}{24Z^{\frac{7}{2}}}. \tag{20}$$

The symmetry $\Gamma_{\alpha\beta\gamma} = \Gamma_{\beta\alpha\gamma}$ now gives

$$\Gamma_{xxz} = \frac{19\kappa\xi\epsilon}{24Z^{\frac{7}{2}}} - \Gamma_{xzx} = \frac{19\kappa\xi\epsilon}{24Z^{\frac{7}{2}}} - \Gamma_{zxx} = \frac{\kappa\xi}{Z^{\frac{7}{2}}}(\frac{19\epsilon}{24} + \frac{1}{4}), \tag{21}$$

as well as

$$\Gamma_{zxz} = \Gamma_{zzx} = 0 \tag{22}$$

The Langevin equation corresponding to this is, using the Ito convention,

$$\frac{dV_\alpha}{dt} = -U_\alpha - \frac{\partial\phi(\mathbf{X})}{\partial X_\alpha} + T\frac{\partial\gamma_{\alpha\beta}}{\partial V_\beta} + \eta_\alpha(t) \tag{23}$$

which can be written as

$$\frac{dV_\alpha}{dt} = -U_\alpha - \frac{\partial\phi(\mathbf{X})}{\partial X_\alpha} + T\Gamma_{\alpha\beta\beta} + \eta_\alpha(t), \tag{24}$$

where we use the Einstein summation convention and the noise correlator is given by

$$\langle\eta_\alpha(t)\eta_\beta(t')\rangle = 2T\gamma_{\alpha\beta}\delta(t-t') = 2T[\lambda_{\alpha\beta}(\mathbf{X}) + \Gamma_{\alpha\beta\gamma}(\mathbf{X})V_\gamma)]\delta(t-t'). \tag{25}$$

Putting this together we find

$$\begin{aligned} \frac{dV_z}{dt} &= -V'(Z) - \xi \frac{V_z}{Z^{\frac{3}{2}}} - \frac{21\kappa\xi}{4}\frac{V_z^2}{Z^{\frac{9}{2}}} + \frac{\kappa\xi}{4}\frac{V_x^2}{Z^{\frac{7}{2}}} + T[\frac{21\kappa\xi}{4Z^{\frac{9}{2}}} - \frac{\kappa\xi}{4Z^{\frac{7}{2}}}] + \eta_z(t) \\ \frac{dV_x}{dt} &= -2\xi\epsilon\frac{V_x}{3Z^{\frac{1}{2}}} - \frac{19\kappa\xi\epsilon}{24}\frac{V_zV_x}{Z^{\frac{7}{2}}} + \eta_x(t) \end{aligned} \tag{26}$$

1. Extra acceleration terms

We have the general set of Newton equations equations

$$m_\alpha \dot{v}_\alpha = F_{h\alpha}(\mathbf{v}, \dot{\mathbf{v}}, \mathbf{x}) - \nabla_\alpha \phi(\mathbf{x}) \tag{27}$$

with

$$\dot{x}_\alpha = v_\alpha. \tag{28}$$

The oddity here is that the hydrodynamic forces F_α (drag and lift) depend on the acceleration terms $\dot{\mathbf{v}}$, in fact one has

$$F_{h\alpha}(\mathbf{v}, \dot{\mathbf{v}}, \mathbf{x}) = F_{1h\alpha}(\mathbf{v}, \mathbf{x}) + F_{2h\alpha\beta}(\mathbf{x})\dot{v}_\beta, \tag{29}$$

and the hydrodynamic force due to the acceleration is linear, and the matrix giving the force only depends on the position. The equations can thus be written as

$$M_{\alpha\beta}\dot{v}_\alpha = F_{1h\alpha}(\mathbf{v}, \mathbf{x}) - \nabla_\alpha \phi(\mathbf{x}) \tag{30}$$

where

$$M_{\alpha\beta} = \delta_{\alpha\beta} m_\alpha - F_{2h\alpha\beta}(\mathbf{x}). \tag{31}$$

The explicit second order equations are thus

$$\dot{v}_\alpha = M^{-1}_{\alpha\beta}[F_{1h\beta}(\mathbf{v}, \mathbf{x}) - \nabla_\beta \phi(\mathbf{x})], \tag{32}$$

We now assume that the effect of temperature is to introduce an anti-Ito noise white

$$\langle \eta_\alpha(t)\eta_\beta(t')\rangle = 2T\gamma_{\alpha\beta}\delta(t-t') \tag{33}$$

and a drift TU_α. This is general as it encompasses all possible prescriptions of stochastic calculs. We thus have

$$\dot{v}_\alpha = M^{-1}_{\alpha\beta}[F_{1h\beta}(\mathbf{v}, \mathbf{x}) - \nabla_\beta \phi(\mathbf{x})] + TU_\alpha + \eta_\alpha. \tag{34}$$

This now gives the Fokker-Planck equation

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial v_\alpha}[T\gamma_{\alpha\beta}\frac{\partial}{\partial v_\alpha}P - [M^{-1}_{\alpha\beta}[F_{1h\beta}(\mathbf{v}, \mathbf{x}) - \nabla_\beta\phi(\mathbf{x})] - TU_\alpha]P] - \frac{\partial}{\partial x_\alpha}[v_\alpha P]. \tag{35}$$

The steady state of this equation must be the GB distribution

$$P_0 = \exp(-\beta \sum_\alpha \frac{m_\alpha v_\alpha^2}{2} - \beta\phi(\mathbf{x})). \tag{36}$$

This must work for all ϕ and so one must have that

$$\beta v_\alpha \nabla_\alpha \phi P + \nabla_\beta \phi(\mathbf{x})\frac{\partial}{\partial v_\alpha}[M^{-1}_{\alpha\beta}P] = 0 \tag{37}$$

and so

$$\beta v_\alpha \nabla_\alpha \phi - \beta \nabla_\beta \phi(\mathbf{x}) M^{-1}_{\alpha\beta} m_\alpha v_\alpha + \nabla_\beta \phi(\mathbf{x}) \frac{\partial}{\partial v_\alpha} M^{-1}_{\alpha\beta} = 0. \tag{38}$$

However $M_{\alpha\beta}$ is independent of $\mathbf{v}$ in the case studied here and so the GB distribution cannot be recovered unless

$$M_{\alpha\beta} = \delta_{\alpha\beta} m_\alpha. \tag{39}$$