Time Correlation function

$$C_{i,j}(\tau) = \frac{1}{T-\tau}\int dt\; h_i(t)h_j(t+\tau)$$ Time average

$$C_{i,j}(\tau) = \int dx_t dx_{t+\tau}\; h_i(x_t)h_j(x_{t+\tau})\;\rho(x_t, x_{t+\tau}) = \int dx_t dx_{t+\tau}\; h_i(x_t)h_j(x_{t+\tau})\;\rho(x_t)\rho(x_{t+\tau}|x_t)$$ Ensemble average

$$\rho(x_t) = \frac{e^{-\beta U(\overrightarrow{x})}}{\mathcal{Z}}$$ Boltzmann distribution

$$\rho(x_{t+\tau}|x_t) = \prod_{i=0}^{n}\rho(x_{t+\tau-i\cdot dt}|x_{t+\tau-(i+1)\cdot dt}) \propto \prod_{i=0}^{n} e^{-\beta\Delta F(s)_{t+\tau-(i+1)dt,t+\tau-idt}} = e^{-\beta(F(s_{t+\tau})-F(s_t))}$$ Conditional probability

$\mathcal{N}$ Normalization of conditional probability

$$\tilde{\rho}(x_t) = \frac{e^{-\beta \tilde{U}(\overrightarrow{x})}}{\tilde{\mathcal{Z}}} \qquad \tilde{U}(\overrightarrow{x}) = U(\overrightarrow{x}) + V(\vec{s}(\overrightarrow{x}))$$

Biased Boltzmann distribution

$$V(s) = \frac{1-\gamma}{\gamma} F(s)$$

Deposited bias during well-tempered biased simulation

$$\tilde{F}(s) = F(s) + \frac{1-\gamma}{\gamma} F(s) = F(s) + V(s)$$

Free Energy shape of biased simulation

$$C_{i,j}(\tau) = \int dx_t dx_{t+\tau}\, h_i(x_t) h_j(x_{t+\tau})\, \frac{e^{-\beta(U(x_t) \pm V(s(x_t)))}}{\mathcal{Z}} \frac{e^{-\beta(F(s_{t+\tau}) - F(s_t) \pm V(s_{t+\tau}) \pm V(s_t))}}{\mathcal{N}}$$

$$C_{i,j}(\tau) = \int dx_t dx_{t+\tau}\, h_i(x_t) h_j(x_{t+\tau})\, \frac{e^{-\beta \tilde{U}(x_t)} e^{\beta V(s_t)}}{\mathcal{Z}} \frac{e^{-\beta(\tilde{F}(s_{t+\tau}) - \tilde{F}(s_t))} e^{\beta(V(s_{t+\tau}) - V(s_t))}}{\mathcal{N}} = \int dx_t dx_{t+\tau}\, h_i(x_t) h_j(x_{t+\tau})\, \tilde{\rho}(x_t) \tilde{\rho}(x_{t+\tau} | x_t) \frac{e^{\beta V(s_{t+\tau})}}{\mathcal{Z}\mathcal{N}}$$

$$\mathscr{Z} = \int d\overrightarrow{x} e^{-\beta U(\overrightarrow{x}) \pm \beta V(\vec{s}(\overrightarrow{x}))} = \int_{\text{biased ensamble}} d\overrightarrow{x} e^{\beta V(\vec{s}(\overrightarrow{x}))}$$

$$\mathscr{N} = ?$$

From Metadynamics of paths

$$\mathrm{R}^{N+1} = \mathrm{R}^{N} + \frac{\delta t}{m\nu}\mathrm{F}^{N} + W$$

$$p(\mathrm{R}^{N+1} \,|\, \mathrm{R}^{N}) = \int \mathcal{N}(W; 0, \Sigma)\,\delta\left(W - (\mathrm{R}^{N+1} - \mathrm{R}^{N} - \frac{\delta t}{m\nu}\mathrm{F}^{N})\right) dW$$

$$\Sigma_{ii} = \frac{m_i \nu}{2\beta\delta t} = \beta^{-1} K_{ii}^{-1}$$

$$= \mathcal{N}(\mathrm{R}^{N+1} - \mathrm{R}^{N} - \frac{\delta t}{m\nu}\mathrm{F}^{N}; 0, \Sigma)$$

$$= \det(2\pi\beta^{-1}\mathrm{K}^{-1})^{-\frac{1}{2}} e^{-\frac{\beta}{2}[\mathrm{R}^{N+1} - \mu(\mathrm{R}^{N+1})]\mathrm{K}[\mathrm{R}^{N} - \mu(\mathrm{R}^{N})]}$$