Soft-Core Stillinger Weber(SW) Potential Notes 2

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The SW potential already uses the parameter λ, so I have used μ instead. SW potential consists of 2-body as well as 3-body terms. The singularity problem occurs in 2-body term only. The soft core two body SW potential is given by the following expression:

$$\phi_2 = \mu^n A\epsilon \left(\frac{B}{\alpha_{SW}(1-\mu)^2 + (r/\sigma)^p} - \frac{1}{\alpha_{SW}(1-\mu)^2 + (r/\sigma)^q} \right) exp\left(\frac{\sigma}{r - a\sigma} \right) \tag{1}$$

The force corresponding to this potential is given by:

$$\mathbf{F} = -\nabla\phi_2 = -\frac{\partial\phi_2}{\partial r} . \frac{\mathbf{r}}{r} \tag{2}$$

$$\begin{aligned} &= \mu^n A\epsilon \left(\frac{Bp(r/\sigma)^p}{[\alpha_{SW}(1-\mu)^2 + (r/\sigma)^p]^2} - \frac{q(r/\sigma)^q}{[\alpha_{SW}(1-\mu)^2 + (r/\sigma)^q]^2} \right) exp\left(\frac{\sigma}{r - a\sigma} \right) \frac{\mathbf{r}}{r^2} \\ &+ \mu^n A\epsilon \left(\frac{B}{\alpha_{SW}(1-\mu)^2 + (r/\sigma)^p} - \frac{1}{\alpha_{SW}(1-\mu)^2 + (r/\sigma)^q} \right) exp\left(\frac{\sigma}{r - a\sigma} \right) * \left(\frac{\sigma}{r - a\sigma} \right) \frac{\mathbf{r}}{r} \end{aligned} \tag{3}$$

$$\begin{aligned} &= \frac{A\epsilon\mu^n}{r^2} exp\left(\frac{\sigma}{r - a\sigma} \right) \left[\frac{Bp(r/\sigma)^p}{[\alpha_{SW}(1-\mu)^2 + (r/\sigma)^p]^2} - \frac{q(r/\sigma)^q}{[\alpha_{SW}(1-\mu)^2 + (r/\sigma)^q]^2} \right. \\ &\qquad \left. + \left(\frac{B}{\alpha_{SW}(1-\mu)^2 + (r/\sigma)^p} - \frac{1}{\alpha_{SW}(1-\mu)^2 + (r/\sigma)^q} \right) \frac{\sigma r}{(r - a\sigma)^2} \right] \mathbf{r} \end{aligned} \tag{4}$$

For the calculation of free energy, the term $\frac{d\phi}{d\mu}$ is required. It can be expressed as follows:

$$\begin{aligned} \frac{d\phi}{d\mu} &= exp\left(\frac{\sigma}{r - a\sigma} \right) \left[n\mu^{n-1} A\epsilon \left(\frac{B}{\alpha_{SW}(1-\mu)^2 + (r/\sigma)^p} - \frac{1}{\alpha_{SW}(1-\mu)^2 + (r/\sigma)^q} \right) \right. \\ &\qquad \left. + 2\mu^n A\epsilon B \alpha_{SW}(1-\mu) \left(\frac{B}{[\alpha_{SW}(1-\mu)^2 + (r/\sigma)^p]^2} - \frac{1}{[\alpha_{SW}(1-\mu)^2 + (r/\sigma)^q]^2} \right) \right] \end{aligned} \tag{5}$$

C++ Notations

rinvsq $= \frac{1}{r^2}$

rbysig $= \frac{r}{\sigma}$

rbysigp $=\left(\frac{r}{\sigma}\right)^p$

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rainv $= \dfrac{1}{r - r\sigma}$

rainvsq $=$ rainv . rainv $= \dfrac{1}{(r - r\sigma)^2}$

expo $=$ exp(sigma . rainv) $= exp\left(\dfrac{\sigma}{r - a\sigma}\right)$

denomp $= \alpha(1-\mu)(1-\mu) + rbysigp = [\alpha_{SW}(1-\mu)^2 + (r/\sigma)^p]$

denomq $= \alpha(1-\mu)(1-\mu) + rbysigp = [\alpha_{SW}(1-\mu)^2 + (r/\sigma)^p]$

coef $= \mu^n.rinvsq.A.\epsilon.expo = \dfrac{A\epsilon\mu^n}{r^2} exp\left(\dfrac{\sigma}{r - a\sigma}\right)$

coef2 $= n\mu^{n-1}A\epsilon$

coef3 $= 2\mu^n A\epsilon\alpha_{SW}(1-\mu)$

Thus the force is given by:

$$\mathbf{F} = fforce.\mathbf{r} \tag{6}$$

where fforce is the force factor given by:

$$coef.\left(\frac{B.p.rbysigp}{denomp.denomp} - \frac{q.rbysigq}{denomq.denomq} + \sigma.rainvsq\left(\frac{B}{denomp} - \frac{1}{denomq}\right)\right) \tag{7}$$

And $\frac{d\phi}{d\mu}$ is given by:

$$expo.\left(coef2.\left(\frac{B}{denomp} - \frac{1}{denomq}\right) + coef3.\left(\frac{B}{denomp.denomp} - \frac{1}{denomq.denomq}\right)\right) \tag{8}$$