To be held in Editorial files 6916
"Dynamic simulation of hydrodynamically interacting suspensions"
by J.F. Brady, R.J. Phillips, J.C. Lester & G. Bossis

APPENDIX: EWALD SUM OF THE MOBILITY INTERACTIONS

We record here the real $(\mathbf{M}^{(1)}(\mathbf{r}))$ and reciprocal $(\mathbf{M}^{(2)}(\mathbf{k}))$ space parts of the Ewald summed mobility interactions. Use has been made of Faxén formulae for the velocities of the particles to include the finite size of the particles. The translational velocity/force coupling was first derived by Beenakker (1986); the remaining can be worked out by straightforward, but tedious, calculus. ξ is an inverse length that regulates the speed of convergence of the two sums, $\mathbf{e}$ is a unit vector along the line connecting the particle centers, r is the interparticle separation distance, and $\hat{\mathbf{k}}$ is a unit vector in the reciprocal lattice. All lengths have been nondimensionalized by the particle radius a, and a common normalization of $6\pi\eta a^{\mathrm{n}}$ has been used, where $\mathrm{n} = 1, 2$ or 3 depending on the mobility coupling.

(a) Translational velocity/force, $U - F$, coupling:

$$\begin{aligned} M_{ij}^{(1)}(\mathbf{r}) = \delta_{ij}\Big\{ &\left(\frac{3}{4}\frac{1}{r} + \frac{1}{2}\frac{1}{r^3}\right)\mathrm{erfc}(\xi r) + \frac{1}{\sqrt{\pi}}(4\xi^7 r^4 + 3\xi^3 r^2 \\ &- 20\xi^5 r^2 - \frac{9}{2}\xi + 14\xi^3 + \xi/r^2)e^{-\xi^2 r^2}\Big\} \\ &+ e_i e_j \Big\{\left(\frac{3}{4}\frac{1}{r} - \frac{3}{2}\frac{1}{r^3}\right)\mathrm{erfc}(\xi r) + \frac{1}{\sqrt{\pi}}(-4\xi^7 r^4 - 3\xi^3 r^2 \\ &+ 16\xi^5 r^2 + \frac{3}{2}\xi - 2\xi^3 - 3\xi/r^2)e^{-\xi^2 r^2}\Big\}, \end{aligned} \tag{A1}$$

$$\begin{aligned} M_{ij}^{(2)}(\mathbf{k}) = (\delta_{ij} - \hat{k}_i\hat{k}_j)(1 - k^2/3)(1 + \frac{1}{4}k^2/\xi^2 + \frac{1}{8}k^4/\xi^4)6\pi k^{-2} \\ \mathrm{x}\ \exp(-\frac{1}{4}k^2/\xi^2), \end{aligned} \tag{A2}$$

$$M_{ij}^{(2)}(\mathbf{r} = 0) = \frac{1}{\sqrt{\pi}}(6\xi - \frac{40}{3}\xi^3). \tag{A3}$$

(b) Translational velocity/torque, $U - L$, coupling:

$$\begin{aligned} M_{ij}^{(1)}(\mathbf{r}) = -\frac{3}{8}\epsilon_{lkj}\Big\{ &\left[-\frac{1}{r^3}\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi\left(-\frac{1}{r^2} + 10\xi^2 - 4\xi^4 r^2\right)e^{-\xi^2 r^2}\right]e_k\delta_{il} \\ &+ \left[\frac{1}{r^3}\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(\frac{1}{r^2} - 2\xi^2)e^{-\xi^2 r^2}\right]e_l\delta_{ik}\Big\}, \end{aligned} \tag{A4}$$

$$M_{ij}^{(2)}(\mathbf{k}) = 3\pi(\epsilon_{ikj}\hat{k}_k)(\frac{1}{k} + \frac{1}{4}k/\xi^2 + \frac{1}{8}k^3/\xi^4)\exp(-\frac{1}{4}k^2/\xi^2), \quad (A5)$$

$$M_{ij}^{(2)}(\mathbf{r}=0) = 0. \quad (A6)$$

(c) Rotational velocity/torque, $\Omega - L$, coupling:

$$M_{ij}^{(1)}(\mathbf{r}) = \delta_{ij}\left\{-\frac{3}{8}\frac{1}{r^3}\mathrm{erfc}(\xi r) - \frac{3}{\sqrt{\pi}}(\xi/r^2 + 14\xi^3 - 20\xi^5 r^2 + 4\xi^7 r^4)e^{-\xi^2 r^2}\right\} \quad (A7)$$
$$- \frac{3}{4}e_i e_j\left\{-\frac{3}{2}\frac{1}{r^3}\mathrm{erfc}(\xi r) + \frac{1}{\sqrt{\pi}}(-3\xi/r^2 - 2\xi^3 + 16\xi^5 r^2 - 4\xi^7 r^4)e^{-\xi^2 r^2}\right\}$$

$$M_{ij}^{(2)}(\mathbf{k}) = \frac{3\pi}{2}(\delta_{ij} - \hat{k}_i\hat{k}_j)(1 + \frac{1}{4}k^2/\xi^2 + \frac{1}{8}k^4/\xi^4)\exp(-\frac{1}{4}k^2/\xi^2), \quad (A8)$$

$$M_{ij}^{(2)}(\mathbf{r}=0) = \frac{10}{\sqrt{\pi}}\xi^3. \quad (A9)$$

(d) Translational velocity/stresslet, $U - S$, coupling:

$$M_{ijk}^{(1)}(\mathbf{r}) = \frac{3}{8}\left\{(x_4 + x_5)(e_k\delta_{ij} + e_j\delta_{ik}) + 2x_5(e_i\delta_{jk}) + 2x_6(e_i e_j e_k)\right.$$
$$\left. + \frac{4}{15}\left[(x_1 + x_2)(e_k\delta_{ij} + e_j\delta_{ik}) + 2x_2(e_i\delta_{jk}) + 2x_3(e_i e_j e_k)\right]\right\}, \quad (A10)$$

$$M_{ijk}^{(2)}(\mathbf{k}) = -3\pi(1 - \frac{4}{15}k^2)[\hat{k}_k(\delta_{ij} - \hat{k}_i\hat{k}_j) + \hat{k}_j(\delta_{ik} - \hat{k}_i\hat{k}_k)]$$
$$\mathrm{x}\ (1/k + \frac{1}{4}k/\xi^2 + \frac{1}{8}k^3/\xi^4)\exp(-\frac{1}{4}k^2/\xi^2), \quad (A11)$$

$$M_{ijk}^{(2)}(\mathbf{r}=0) = 0. \quad (A12)$$

where

$$x_1 = -6\frac{1}{r^4}\mathrm{erfc}(\xi r) + \frac{4}{\sqrt{\pi}}(-3\xi/r^3 - 2\xi^3/r - 68\xi^5 r + 56\xi^7 r^3 - 8\xi^9 r^5)e^{-\xi^2 r^2},$$
$$x_2 = 4\left[-\frac{3}{2}\frac{1}{r^4}\mathrm{erfc}(\xi r) + \frac{1}{\sqrt{\pi}}(-3\xi/r^3 - 2\xi^3/r + 16\xi^5 r - 4\xi^7 r^3)e^{-\xi^2 r^2}\right],$$

$$x_3 = 4\left[\frac{15}{2}\frac{1}{r^4}\mathrm{erfc}(\xi r) + \frac{1}{\sqrt{\pi}}(15\xi/r^3 + 10\xi^3/r + 4\xi^5 r - 40\xi^7 r^3 + 8\xi^9 r^5)e^{-\xi^2 r^2}\right],$$

$$x_4 = -\frac{1}{r^2}\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(-1/r + 10\xi^2 r - 4\xi^4 r^3)e^{-\xi^2 r^2},$$

$$x_5 = \frac{1}{r^2}\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(1/r - 2\xi^2 r)e^{-\xi^2 r^2}, \qquad (A13)$$

$$x_6 = -\frac{3}{r^2}\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(-3/r - 2\xi^2 r + 4\xi^4 r^3)e^{-\xi^2 r^2}.$$

(e) Rotational velocity/stresslet, $\Omega - S$, coupling:

$$M^{(1)}_{ijk}(\mathbf{r}) = -\frac{3}{16}(y_2 - y_1)[\hat{k}_k(\hat{k}_l\epsilon_{lij}) + \hat{k}_j(\hat{k}_l\epsilon_{lik})], \qquad (A14)$$

$$M^{(2)}_{ijk}(\mathbf{k}) = -\frac{3\pi}{2}[\hat{k}_k(\hat{k}_l\epsilon_{lij})] + \hat{k}_j(\hat{k}_l\epsilon_{lik})](1 + \frac{1}{4}k^2/\xi^2 + \frac{1}{8}k^4/\xi^4)$$
$$\text{x}\ \exp(-\frac{1}{4}k^2/\xi^2), \qquad (A15)$$

$$M^{(2)}_{ijk}(\mathbf{r}=0) = 0, \qquad (A16)$$

where

$$y_1 = \frac{3}{r^3}\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(3/r^2 + 2\xi^2 - 28\xi^4 r^2 + 8\xi^6 r^4)e^{-\xi^2 r^2},$$

$$y_2 = -\frac{3}{r^3}\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(3/r^2 - 2\xi^2 + 4\xi^4 r^2)e^{-\xi^2 r^2}. \qquad (A17)$$

(f) Rate of strain/stresslet, $E - S$, coupling:

$$M^{(1)}_{iljk}(\mathbf{r}) = -\frac{3}{16}r^2 M^{(1A)}_{iljk}(\mathbf{r}) - \frac{3}{80}M^{(1B)}_{iljk}(\mathbf{r}), \qquad (A18)$$

$$M^{(2)}_{iljk}(\mathbf{k}) = \frac{3\pi}{2}(1 - \frac{1}{5}k^2)[\hat{k}_l\hat{k}_k(\delta_{ij} - \hat{k}_i\hat{k}_j) + \hat{k}_l\hat{k}_j(\delta_{ik} - \hat{k}_i\hat{k}_k)$$
$$+ \hat{k}_i\hat{k}_k(\delta_{lj} - \hat{k}_l\hat{k}_j) + \hat{k}_i\hat{k}_j(\delta_{lk} - \hat{k}_l\hat{k}_k)](1 + \frac{1}{4}k^2/\xi^2$$
$$+ \frac{1}{8}k^4/\xi^4)\exp(-\frac{1}{4}k^2/\xi^2), \qquad (A19)$$

$$M^{(2)}_{iljk}(\mathbf{r}=0) = \frac{3}{\sqrt{\pi}}\left(2\xi^3 - \frac{126}{25}\xi^5\right)\left(\delta_{ij}\delta_{lk} + \delta_{ik}\delta_{lj} - \frac{2}{3}\delta_{il}\delta_{jk}\right), \qquad (A20)$$

where

$$M^{(1A)}_{iljk}(\mathbf{r}) = 2(z_3 + z_1)(\delta_{lk}\delta_{ij} + \delta_{jl}\delta_{ik}) + 4z_3\delta_{jk}\delta_{il}$$
$$+ (z_2 + 3z_4)(\delta_{ij}e_le_k + \delta_{jl}e_ie_k + \delta_{lk}e_ie_j + \delta_{ik}e_je_l) \quad (A21)$$
$$+ 4z_4(\delta_{il}e_je_k + \delta_{jk}e_ie_l) + 4z_5e_ie_je_ke_l,$$

$$M^{(1B)}_{iljk}(\mathbf{r}) = 2(D2z_1 + 2z_2 + 6z_4 + D2z_3)(\delta_{jl}\delta_{ki} + \delta_{kl}\delta_{ij})$$
$$+ 4(D2z_3 + 4z_4)\delta_{jk}\delta_{il} + 4(D2z_4 + 2z_5 + 4Dz_4)(\delta_{il}e_ke_j + \delta_{jk}e_ie_l)$$
$$+ \left[3(D2z_4 + 2z_5 + 4Dz_4) + 4Dz_2 + D2z_2 + 2z_5\right](\delta_{ik}e_je_l$$
$$+ \delta_{kl}e_ie_j + \delta_{jl}e_ie_k + \delta_{ij}e_ke_l) + 4(8Dz_5 + D2z_5)e_ie_je_ke_l, \quad (A22)$$

and

$$z_1 = -1/r^5\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(-1/r^4 + 10\xi^2/r^2 - 4\xi^4)e^{-\xi^2r^2}$$
$$z_2 = 3/r^5\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(3/r^4 - 28\xi^4 + 2\xi^2/r^2 + 8\xi^6r^2)e^{-\xi^2r^2}$$
$$z_3 = 1/r^5\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(1/r^4 - 2\xi^2/r^2)e^{-\xi^2r^2}$$
$$z_4 = -3/r^5\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(-3/r^4 - 2\xi^2/r^2 + 4\xi^4)e^{-\xi^2r^2}$$
$$z_5 = 15/r^5\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(15/r^4 + 10\xi^2/r^2 + 4\xi^4 - 8\xi^6r^2)e^{-\xi^2r^2}$$
$$Dz_1 = 3/r^5\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(3/r^4 - 8\xi^4 + 2\xi^2/r^2 - 20\xi^4 + 8\xi^6r^2)e^{-\xi^2r^2}$$
$$Dz_2 = -15/r^5\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(-15/r^4 - 10\xi^2/r^2 + 72\xi^6r^2 - 4\xi^4 - 16\xi^8r^4)e^{-\xi^2r^2}$$
$$Dz_3 = -3/r^5\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(-3/r^4 - 2\xi^2/r^2 + 4\xi^4)e^{-\xi^2r^2}$$
$$Dz_4 = 15/r^5\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(15/r^4 + 10\xi^2/r^2 + 4\xi^4 - 8\xi^6r^z)e^{-\xi^2r^2}$$
$$Dz_5 = -105/r^5\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(-105/r^4 - 70\xi^z/r^2 - 28\xi^4 - 8\xi^6r^2 + 16\xi^8r^4)e^{-\xi^2r^2}$$
$$D2z_1 = -6/r^5\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(-6/r^4 - 88\xi^4 - 4\xi^2/r^2 + 96\xi^6r^2 - 16\xi^8r^4)e^{-\xi^2r^2}$$
$$D2z_2 = 60/r^5\mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(60/r^4 + 40\xi^2/r^2 + 224\xi^6r^2 + 16\xi^4 - 224\xi^8r^4$$

$$+32\xi^{10}r^6)e^{-\xi^2 r^2}$$

$$D2z_3 = 6/r^5 \mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(6/r^4 + 4\xi^2/r^2 + 16\xi^4 - 8\xi^6 r^2)e^{-\xi^2 r^2}$$

$$D2z_4 = -60/r^5 \mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(-60/r^4 - 40\xi^2/r^2 - 16\xi^4 - 32\xi^6 r^2 + 16\xi^8 r^4)e^{-\xi^2 r^2}$$

$$D2z_5 = 630/r^5 \mathrm{erfc}(\xi r) + \frac{2}{\sqrt{\pi}}\xi(630/r^4 + 420\xi^2/r^2 + 168\xi^4 + 48\xi^6 r^2$$

$$+649^8 r^4 - 32\xi^{10}r^6)e^{-\xi^2 r^2}$$

Finally, to include the mean field quadrupole, the finite size contributions to the $U - F$ couplings are replaced by $1 - \frac{1}{5}\phi$, i.e. in (A1), (A2) and (A3), all terms that would have units of $(\text{length})^{-3}$ if written in dimensional form.