Python results Hamaker coefficients for perpendicular [6,5], [9,0], [9,1], [9,3], and [29,0] cylinders in water using retarded and non-retarded formulations.

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Abstract

Comparison of contributions of Matsubara sums to the retarded formulation for
Hamaker coeffiecient, $\mathcal{A}^{(0)}$. I choose to use [6,5], a semiiconductor,
and [9,3], a semimetal, as examples. All caluclations are for identical pairs of
CNTs in water with a mutual angle of $\pi/2$.

Equations correspond to those in version 4 of Rudi's report.

Contents

1 CNTs

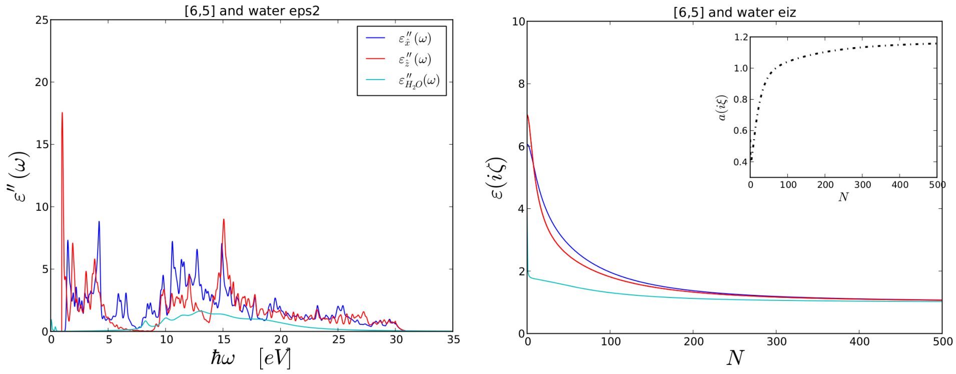
1.1 [6,5] Dielectric response spectrum, dispersion spectrum, and anisotropy measure

From the imaginary part of the dielectric response function of the carbon nanotubes,
we compute the London dispersion spectrum by the Kramers-Kronig transform:

$$\epsilon(i\zeta_n) = 1 + \frac{\pi}{2}\int_0^\infty dw\ \frac{\epsilon\prime\prime(\omega)\omega}{\omega^2+\zeta^2} \tag{1}$$

Relative anisotropy measures in the parallel and perpendicular direction are given by

$$\Delta_\perp = \frac{{\epsilon^c}_\perp - \epsilon_m}{{\epsilon^c}_\perp + \epsilon_m} \qquad \Delta_\parallel = \frac{{\epsilon^c}_\parallel - \epsilon_m}{\epsilon_m}. \tag{2}$$



(a) (b)

Figure 1: (a) Imaginary dielectric response spectrum, (b) dispersion spectrum and anisotropy measure (inset)

Ratio of anisotropy measure:

$$a_{1,2}(i\omega_n) = \frac{2\Delta_{\perp}^{(1,2)}(i\omega_n)}{\Delta_{\parallel}^{(1,2)}(i\omega_n)} = 2\frac{({\epsilon^c}_{\perp}{}^{(1,2)}(i\omega_n) - \epsilon_m(i\omega_n))\epsilon_m(i\omega_n)}{({\epsilon^c}_{\perp}{}^{(1,2)}(i\omega_n) + \epsilon_m(i\omega_n))({\epsilon^c}_{\parallel}{}^{(1,2)}(i\omega_n) - \epsilon_m(i\omega_n))} \tag{3}$$

For interactions between identical CNTs, we set $a_1 = a_2$.

2 [9,0] dielectric response spectrum, dispersion spectrum, and anisotropy measure

Relative anisotropy measures in the parallel and perpendicular direction are given by

$$\Delta_{\perp} = \frac{{\epsilon^c}_{\perp} - \epsilon_m}{{\epsilon^c}_{\perp} + \epsilon_m} \qquad \Delta_{\parallel} = \frac{{\epsilon^c}_{\parallel} - \epsilon_m}{\epsilon_m}. \tag{4}$$

Ratio of anisotropy measures

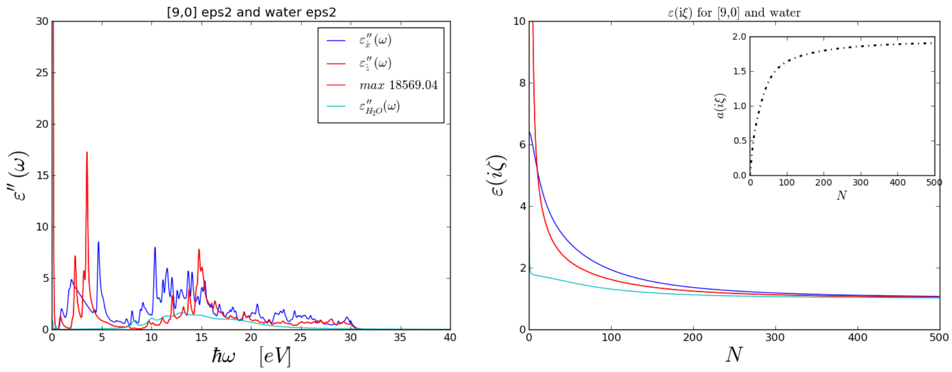
$$a_{1,2}(i\omega_n) = \frac{2\Delta_{\perp}^{(1,2)}(i\omega_n)}{\Delta_{\parallel}^{(1,2)}(i\omega_n)} =$$

$$2\;(\epsilon^c_{\perp}{}^{(1,2)}(i\omega_n) - \epsilon_m(i\omega_n))\epsilon_m(i\omega_n)\frac{}{({\epsilon^c}_{\perp}{}^{(1,2)}(i\omega_n)+\epsilon_m(i\omega_n))({\epsilon^c}_{\parallel}{}^{(1,2)}(i\omega_n)-\epsilon_m(i\omega_n))} \tag{5}$$

3 [9,1] dielectric response spectrum, dispersion spectrum, and anisotropy measure

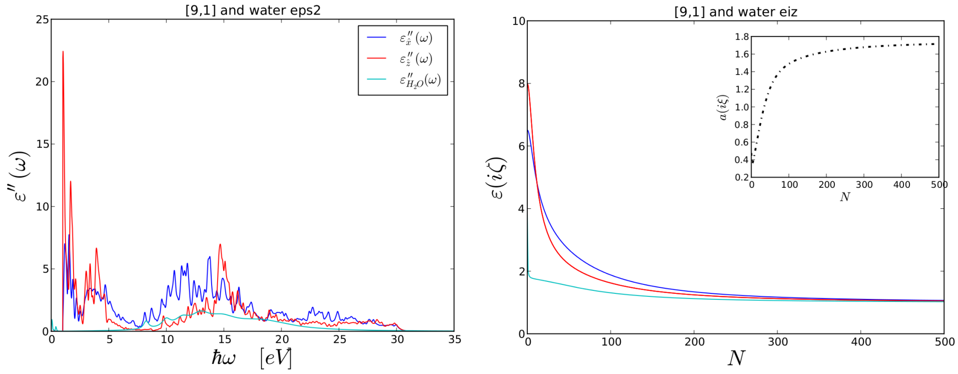
Relative anisotropy measures in the parallel and perpendicular direction are given by

$$\Delta_{\perp} = \frac{{\epsilon^c}_{\perp} - \epsilon_m}{{\epsilon^c}_{\perp} + \epsilon_m} \qquad \Delta_{\parallel} = \frac{{\epsilon^c}_{\parallel} - \epsilon_m}{\epsilon_m}. \tag{6}$$



(a) (b)

Figure 2: (a) Imaginary dielectric response spectrum, (b) dispersion spectrum and anistropy measure (inset)



(a) (b)

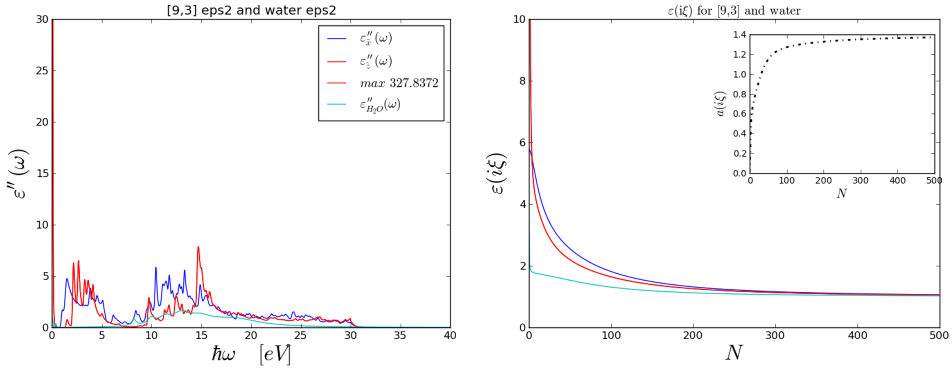
Figure 3: (a) Imaginary dielectric response spectrum, (b) dispersion spectrum and anistropy measure (inset)

Ratio of anisotropy measures

$$a_{1,2}(i\omega_n) = \frac{2\Delta_{\perp}^{(1,2)}(i\omega_n)}{\Delta_{\parallel}^{(1,2)}(i\omega_n)} = 2\frac{({\epsilon^c}_{\perp}{}^{(1,2)}(i\omega_n) - \epsilon_m(i\omega_n))\epsilon_m(i\omega_n)}{({\epsilon^c}_{\perp}{}^{(1,2)}(i\omega_n) + \epsilon_m(i\omega_n))({\epsilon^c}_{\parallel}{}^{(1,2)}(i\omega_n) - \epsilon_m(i\omega_n))} \tag{7}$$

4 [9,3] dielectric response spectrum, dispersion spectrum, and anisotropy measure

Relative anisotropy measures in the parallel and perpendicular direction are given by



(a)

(b)

Figure 4: (a) Imaginary dielectric response spectrum, (b) dispersion spectrum and anistropy measure (inset)

$$\Delta_\perp = \frac{{\epsilon^c}_\perp - \epsilon_m}{{\epsilon^c}_\perp + \epsilon_m} \qquad \Delta_\parallel = \frac{{\epsilon^c}_\parallel - \epsilon_m}{\epsilon_m}. \tag{8}$$

Ratio of anisotropy measures

$$a_{1,2}(i\omega_n) = \frac{2\Delta_\perp^{(1,2)}(i\omega_n)}{\Delta_\parallel^{(1,2)}(i\omega_n)} = 2\frac{({\epsilon^c}_\perp^{(1,2)}(i\omega_n) - \epsilon_m(i\omega_n))\epsilon_m(i\omega_n)}{({\epsilon^c}_\perp^{(1,2)}(i\omega_n) + \epsilon_m(i\omega_n))({\epsilon^c}_\parallel^{(1,2)}(i\omega_n) - \epsilon_m(i\omega_n))} \tag{9}$$

5 [29,0] dielectric response spectrum, dispersion spectrum, and anisotropy measure

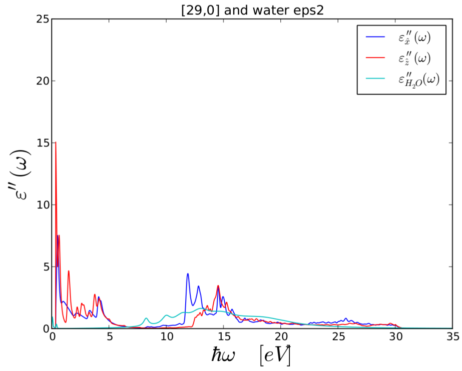
Relative anisotropy measures in the parallel and perpendicular direction are given by

$$\Delta_\perp = \frac{{\epsilon^c}_\perp - \epsilon_m}{{\epsilon^c}_\perp + \epsilon_m} \qquad \Delta_\parallel = \frac{{\epsilon^c}_\parallel - \epsilon_m}{\epsilon_m}. \tag{10}$$

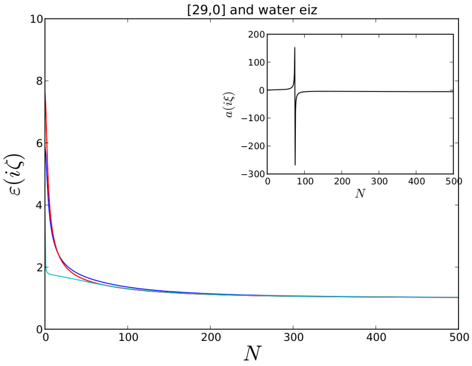
Ratio of anisotropy measures

$$a_{1,2}(i\omega_n) = \frac{2\Delta_\perp^{(1,2)}(i\omega_n)}{\Delta_\parallel^{(1,2)}(i\omega_n)} = 2\frac{({\epsilon^c}_\perp^{(1,2)}(i\omega_n) - \epsilon_m(i\omega_n))\epsilon_m(i\omega_n)}{({\epsilon^c}_\perp^{(1,2)}(i\omega_n) + \epsilon_m(i\omega_n))({\epsilon^c}_\parallel^{(1,2)}(i\omega_n) - \epsilon_m(i\omega_n))} \tag{11}$$

Fully retarded Hamaker Coefficients for Matsubara Sum



(a)



(b)

Figure 5: (a) Imaginary dielectric response spectrum, (b) dispersion spectrum and anisotropy measure (inset)

6 Semi-conductor [6,5]

6.1 [6,5] terms of Matsubara sum

We write the Hamaker coefficients as,

$$\mathcal{A}^{(0)}(\ell) = \frac{k_B T}{32} {\sum_{n=0}^{\infty}}' \Delta_{1,\parallel} \Delta_{2,\parallel} \, p_n^4(\ell) \int_0^\infty t dt \, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{12}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) = \\ 2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right]$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_B T}{32} {\sum_{n=0}^{\infty}}' \Delta_{1,\parallel} \Delta_{2,\parallel} \, p_n^4(\ell) \int_0^\infty t dt \, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{13}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2$$

Where

$$p_n^2(\ell) = \epsilon_m(i\omega_n)\frac{\omega_n^2}{c^2}\ell^2,$$

$$\Delta_\perp = \frac{{\epsilon^c}_\perp - \epsilon_m}{{\epsilon^c}_\perp + \epsilon_m} \qquad \Delta_\parallel = \frac{{\epsilon^c}_\parallel - \epsilon_m}{\epsilon_m},$$

$$a = \frac{2\Delta_\perp}{\Delta_\parallel} = 2\frac{({\epsilon^c}_\perp - \epsilon_m)\epsilon_m}{({\epsilon^c}_\perp + \epsilon_m)({\epsilon^c}_\parallel - \epsilon_m)}$$

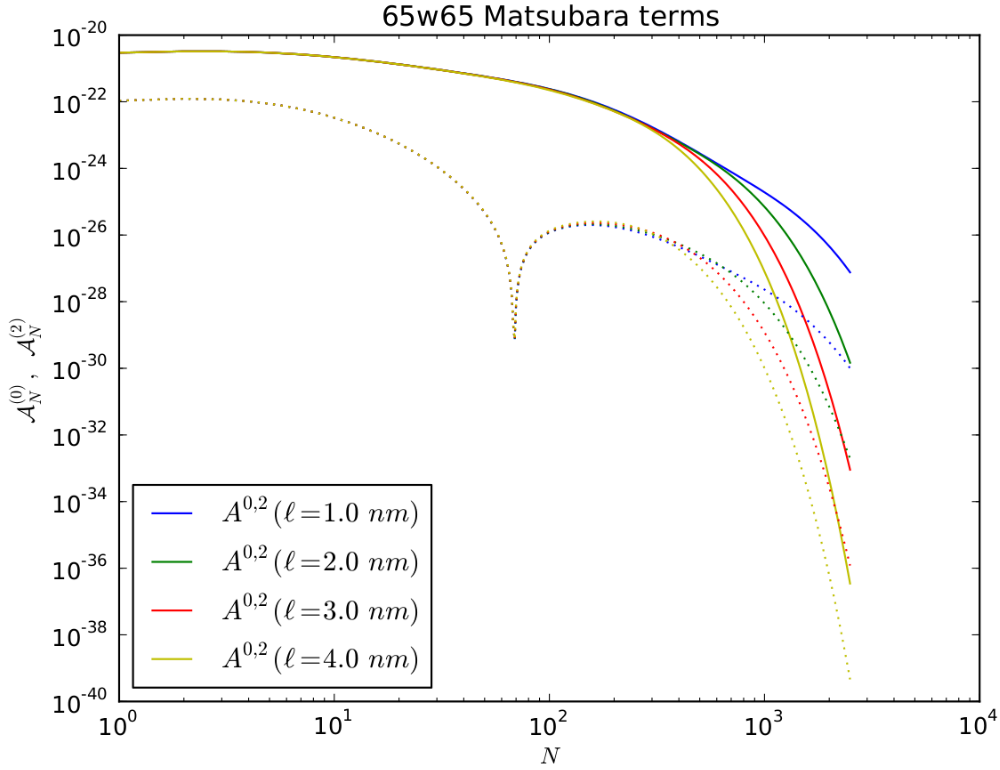


Figure 6: Terms contributing to Matsubara sum as a function of N

For n = 0, we use

$$\mathcal{A}^{(0)}_{n=0}(\ell) = \frac{1}{2}\frac{k_BT}{32}\Delta_{1,\|}\Delta_{2,\|}\int_0^\infty u^3du\; e^{-2u}\;[2(1+3a_1)(1+3a_2)] \tag{14}$$

and

$$\mathcal{A}^{(2)}_{n=0}(\ell) = \frac{1}{2}\frac{k_BT}{32}\Delta_{1,\|}\Delta_{2,\|}\int_0^\infty u^3du\; e^{-2u}\;[(1-a_1)(1-a_2)] \tag{15}$$

where $u = Ql$.

6.2 [6,5] Log-log plot of $\mathcal{A}^{(0)}$ and $\mathcal{A}^{(2)}$

$$\mathcal{A}^{(0)}(\ell) = \frac{k_BT}{32}{\sum_{n=0}^{\infty}}{}' \Delta_{1,\|}\Delta_{2,\|}\; p_n^4(\ell)\int_0^\infty tdt\;\frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)}\tilde{g}^{(0)}(t,a_1(i\omega_n),a_2(i\omega_n)) \tag{16}$$

with

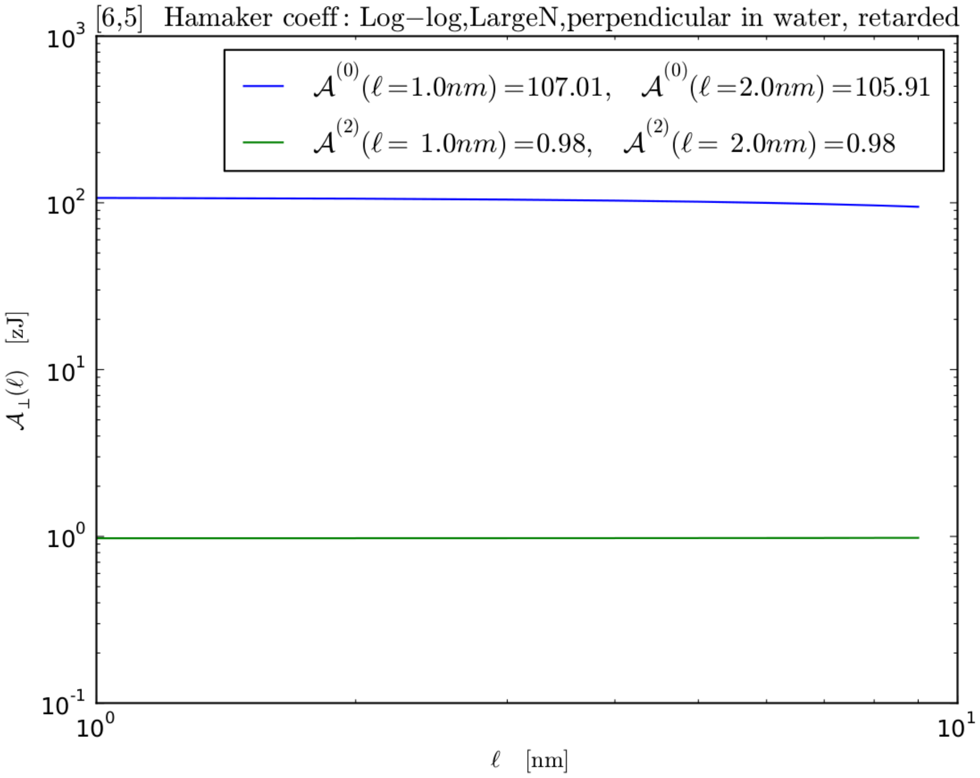


Figure 7: Full result

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) =$$
$$2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right]$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_BT}{32}{\sum_{n=0}^{\infty}}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{17}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{18}$$

6.3 [6,5] Semi-log plot of $\mathcal{A}^{(0)}$ and $\mathcal{A}^{(2)}$

$$\mathcal{A}^{(0)}(\ell) = \frac{k_B T}{32} \sum_{n=0}^{\infty}{}' \Delta_{1,\|}\Delta_{2,\|}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{19}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) = \\ 2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right]$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_B T}{32} \sum_{n=0}^{\infty}{}' \Delta_{1,\|}\Delta_{2,\|}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{20}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{21}$$

7 Semi-conductor [9,1]

7.1 [9,1] terms of Matsubara sum

$$\mathcal{A}^{(0)}(\ell) = \frac{k_B T}{32} \sum_{n=0}^{\infty}{}' \Delta_{1,\|}\Delta_{2,\|}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{22}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) = \\ 2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right]$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_B T}{32} \sum_{n=0}^{\infty}{}' \Delta_{1,\|}\Delta_{2,\|}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{23}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{24}$$

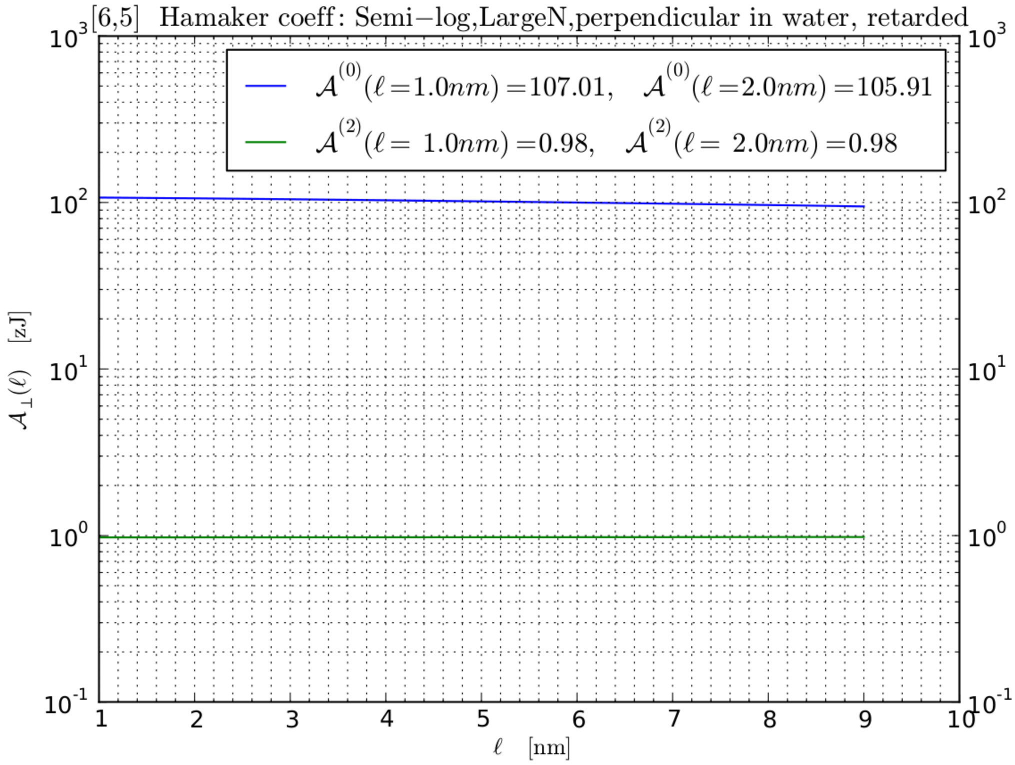


Figure 8: Full result

7.2 [9,1] Log-log plot of $\mathcal{A}^{(0)}$ and $\mathcal{A}^{(2)}$

$$\mathcal{A}^{(0)}(\ell) = \frac{k_BT}{32}\sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)}\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{25}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) =$$
$$2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right]$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_BT}{32}\sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)}\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{26}$$

with

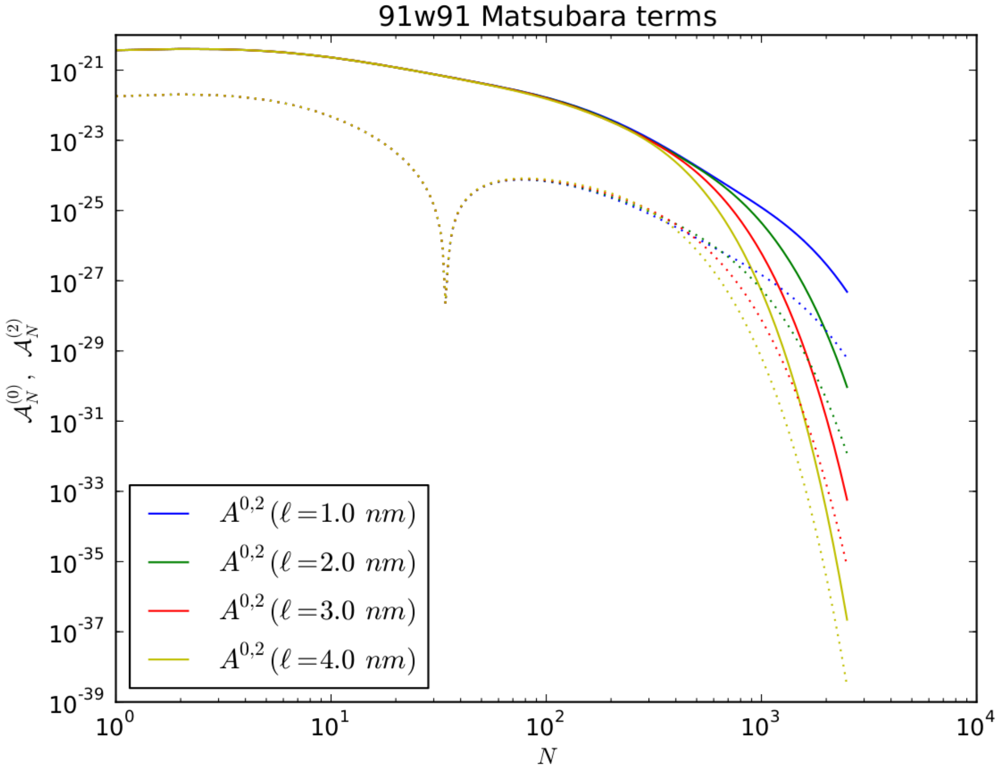


Figure 9: Terms contributing to Matsubara sum as a function of N

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1 - a_1)(1 - a_2)(t^2 + 2)^2 \tag{27}$$

7.3 [9,1] Semi-log plot of $\mathcal{A}^{(0)}$ and $\mathcal{A}^{(2)}$

$$\mathcal{A}^{(0)}(\ell) = \frac{k_B T}{32} \sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{28}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) =$$
$$2\left[(1 + 3a_1)(1 + 3a_2)t^4 + 2(1 + 2a_1 + 2a_2 + 3a_1a_2)t^2 + 2(1 + a_1)(1 + a_2)\right]$$

and

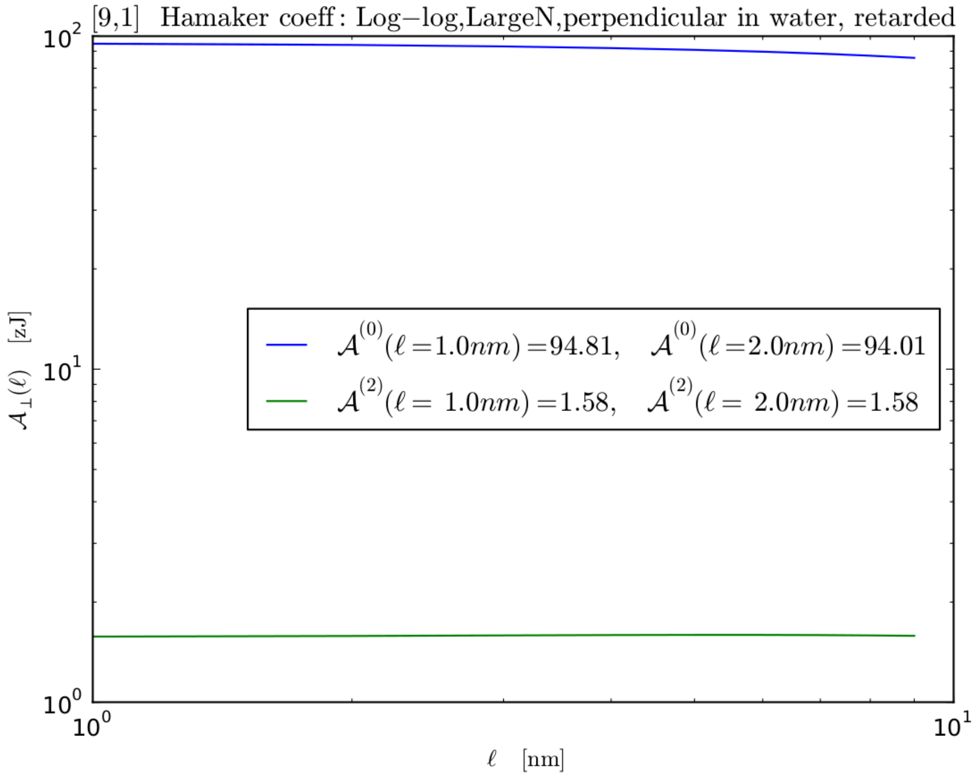


Figure 10: Full result

$$\mathcal{A}^{(2)}(\ell) = \frac{k_BT}{32}\sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell)\, \int_0^\infty tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)}\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{29}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{30}$$

8 First results for semi-metal [9,3]

8.1 [9,3] terms of unmodified Matsubara sum

$$\mathcal{A}^{(0)}(\ell) = \frac{k_BT}{32}\sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell)\, \int_0^\infty tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)}\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{31}$$

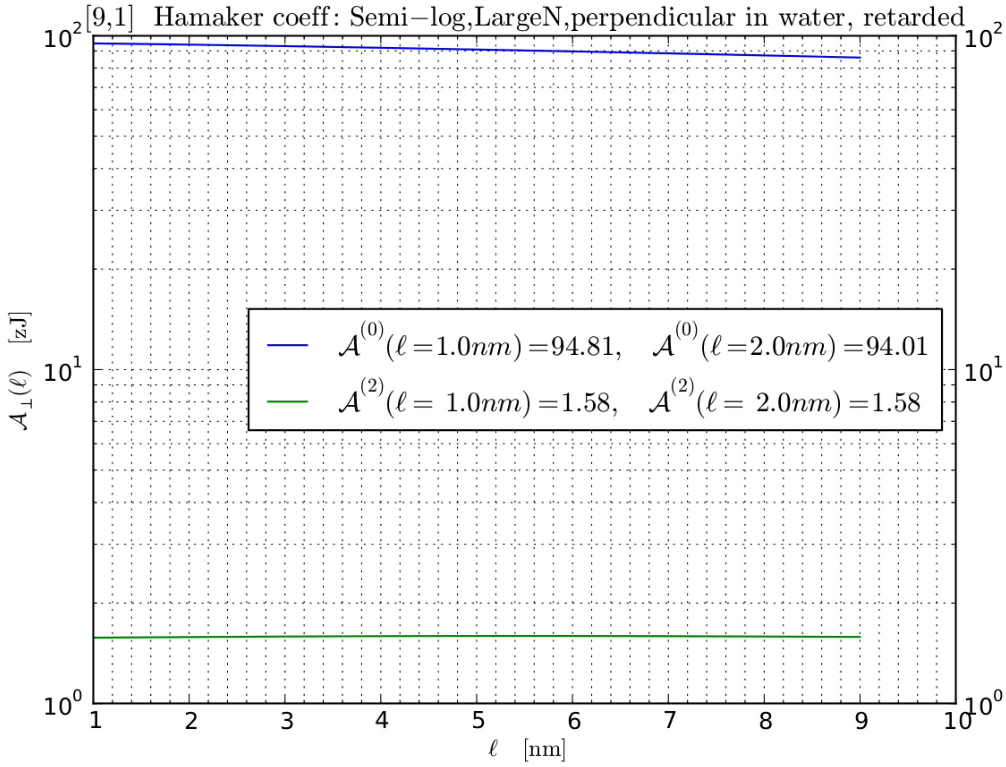


Figure 11: Full result

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) =$$
$$2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right]$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_BT}{32}{\sum_{n=0}^{\infty}}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{32}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{33}$$

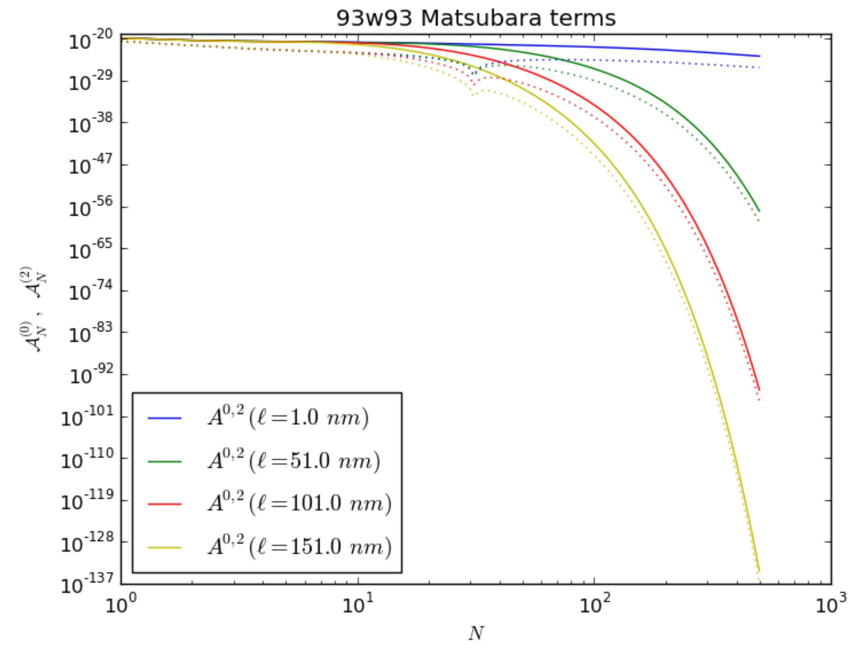


Figure 12: Full result

8.2 [9,3] terms of modified Matsubara sum with $\mathcal{A}(n=0)=0$

$$\mathcal{A}^{(0)}(\ell) = \frac{k_B T}{32} {\sum_{n=0}^{\infty}}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{34}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) = 2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right] \tag{35}$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_B T}{32} {\sum_{n=0}^{\infty}}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{36}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{37}$$

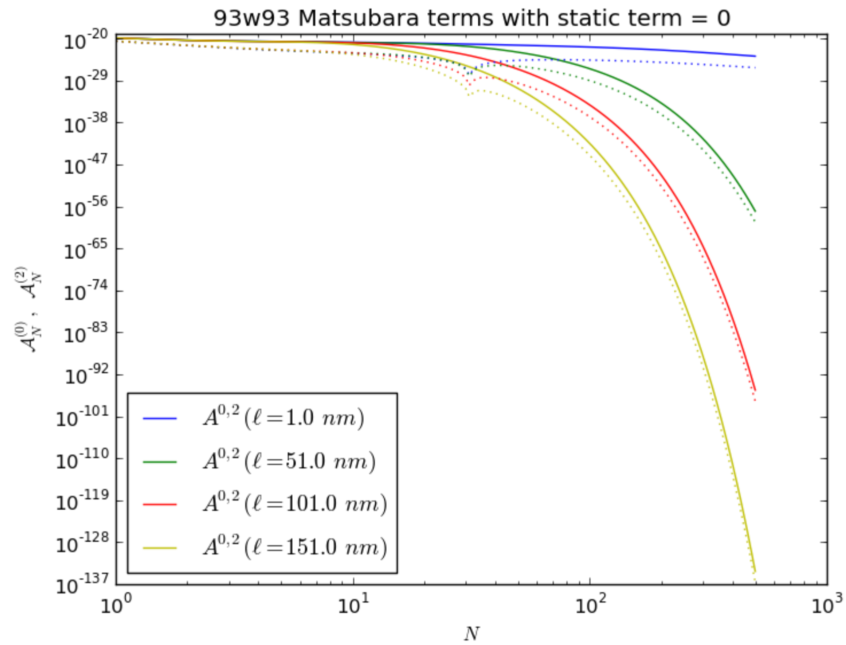


Figure 13: Full result

8.3 [9,3] Log-log plot of unmodified $\mathcal{A}$

$$\mathcal{A}^{(0)}(\ell) = \frac{k_BT}{32}\sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)}\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{38}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) =$$
$$2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right]$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_BT}{32}\sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)}\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{39}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{40}$$

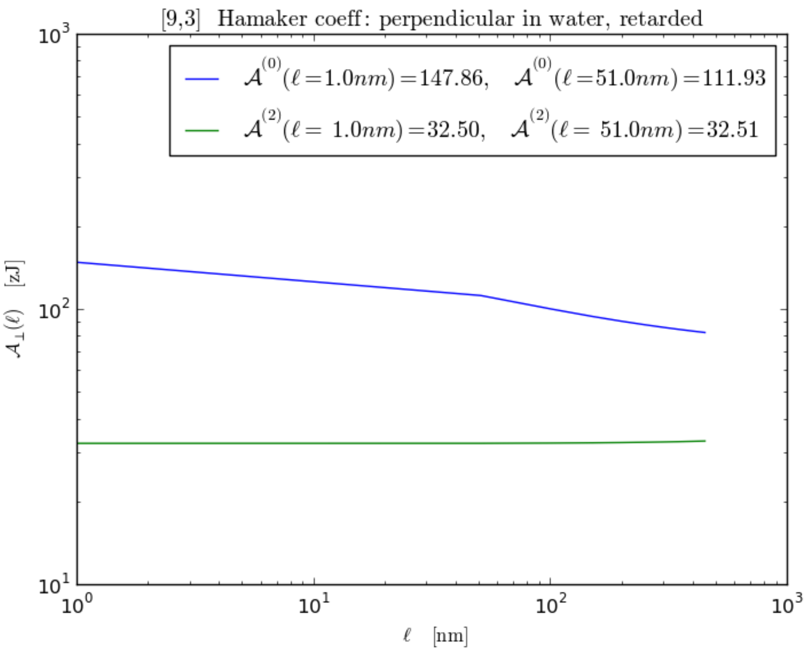


Figure 14: Full result

8.4 [9,3] Log-log plot of modified $\mathcal{A}(n=0)=0$

$$\mathcal{A}^{(0)}(\ell) = \frac{k_B T}{32} \sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{41}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) = \\ 2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right]$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_B T}{32} \sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{42}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{43}$$

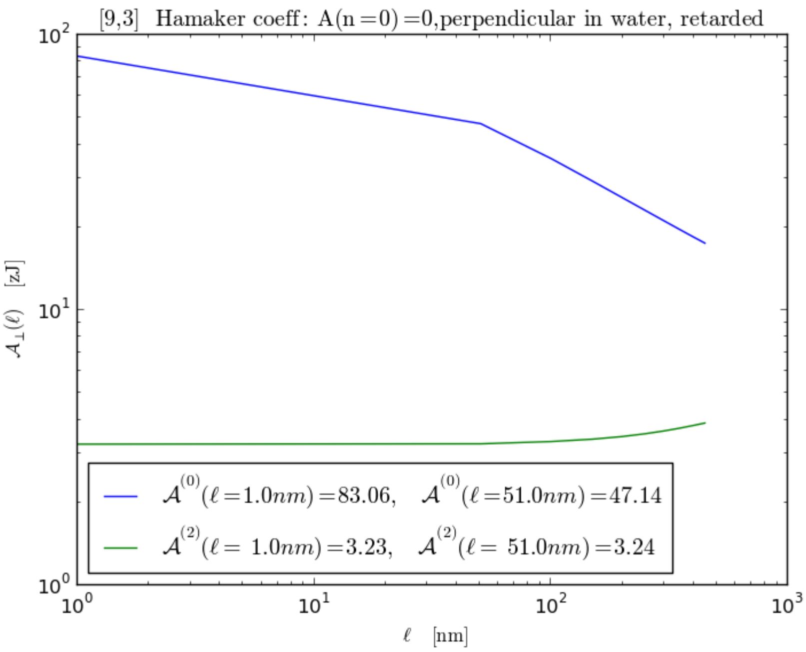


Figure 15: Full result

8.5 [9,3] Semi-log plot of unmodified $\mathcal{A}$

$$\mathcal{A}^{(0)}(\ell) = \frac{k_BT}{32}\sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell)\ \int_0^\infty t dt\ \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)}\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{44}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) =$$
$$2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right]$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_BT}{32}\sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell)\ \int_0^\infty t dt\ \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)}\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{45}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{46}$$

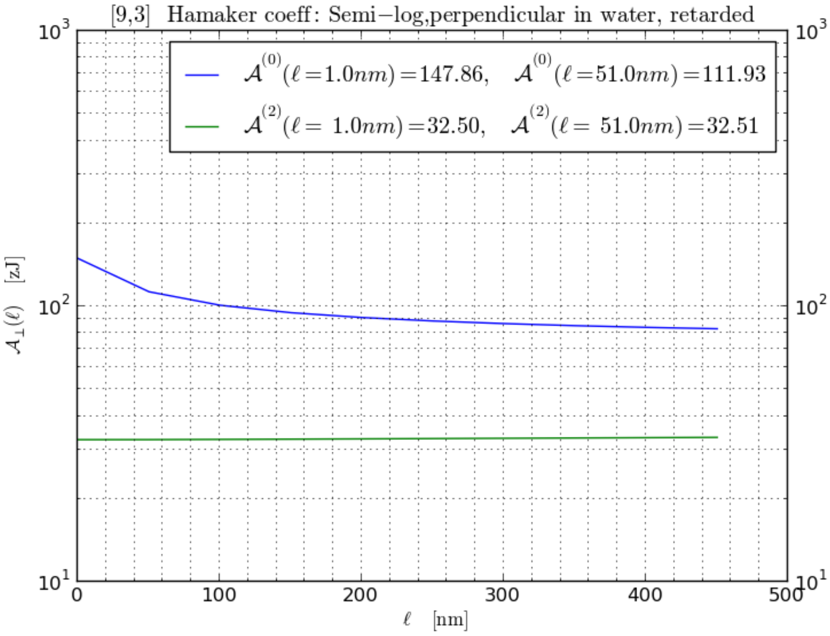


Figure 16: Full result

8.6 [9,3] Semi-log plot of modified $\mathcal{A}(n=0)=0$

$$\mathcal{A}^{(0)}(\ell) = \frac{k_BT}{32}\sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{47}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) = 2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right]$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_BT}{32}\sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{48}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{49}$$

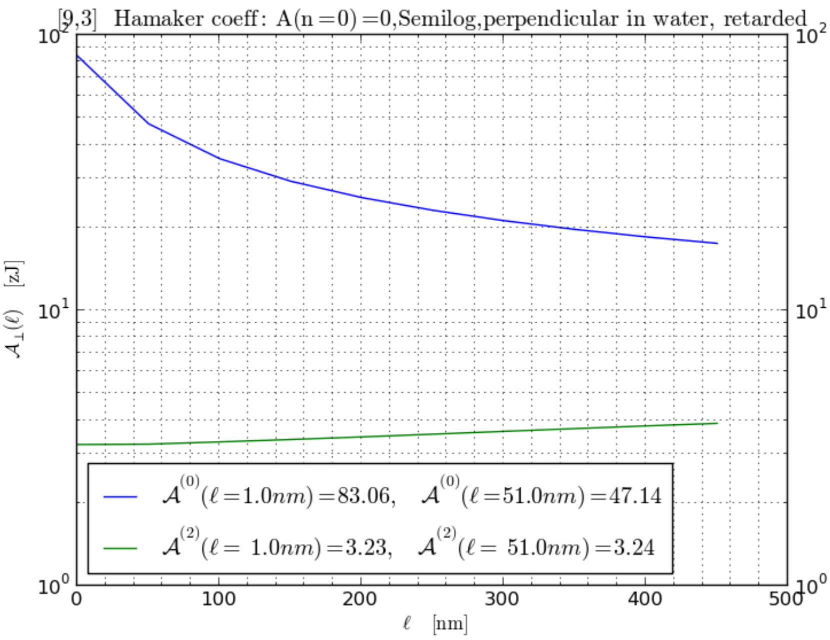


Figure 17: Full result

9 Semi-conductor [29,0]

9.1 [29,0] terms of Matsubara sum

$$\mathcal{A}^{(0)}(\ell) = \frac{k_B T}{32} \sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{50}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) = \\ 2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right]$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_B T}{32} \sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{51}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{52}$$

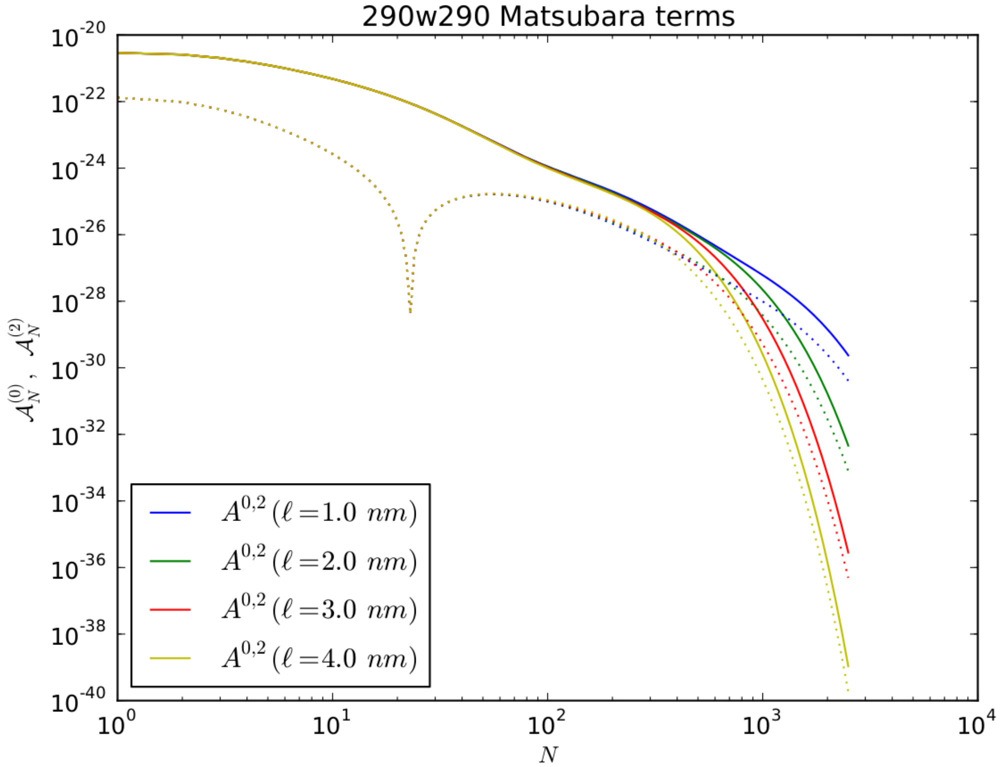


Figure 18: Full result

9.2 [29,0] Log-log plot of $\mathcal{A}^{(0)}$ and $\mathcal{A}^{(2)}$

$$\mathcal{A}^{(0)}(\ell) = \frac{k_B T}{32} {\sum_{n=0}^{\infty}}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell)\, \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{53}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) = \\ 2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right]$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_B T}{32} {\sum_{n=0}^{\infty}}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell)\, \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{54}$$

with

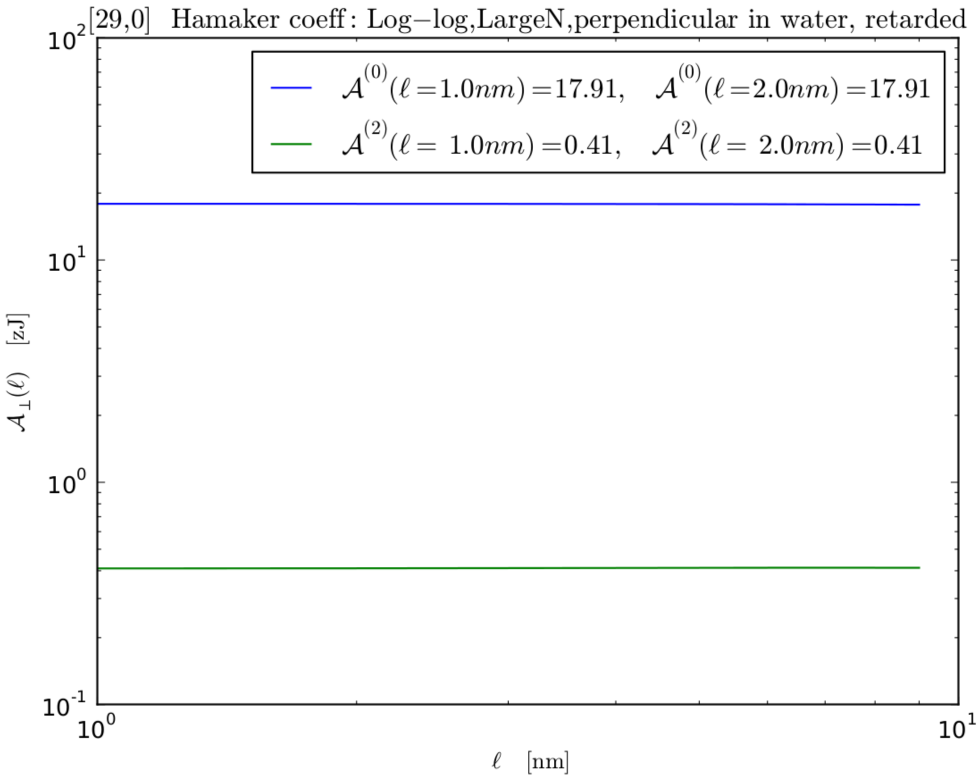


Figure 19: Full result

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1 - a_1)(1 - a_2)(t^2 + 2)^2 \tag{55}$$

9.3 [29,0] Semi-log plot of $\mathcal{A}^{(0)}$ and $\mathcal{A}^{(2)}$

$$\mathcal{A}^{(0)}(\ell) = \frac{k_B T}{32} \sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{56}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) =$$
$$2\left[(1 + 3a_1)(1 + 3a_2)t^4 + 2(1 + 2a_1 + 2a_2 + 3a_1a_2)t^2 + 2(1 + a_1)(1 + a_2)\right]$$

and

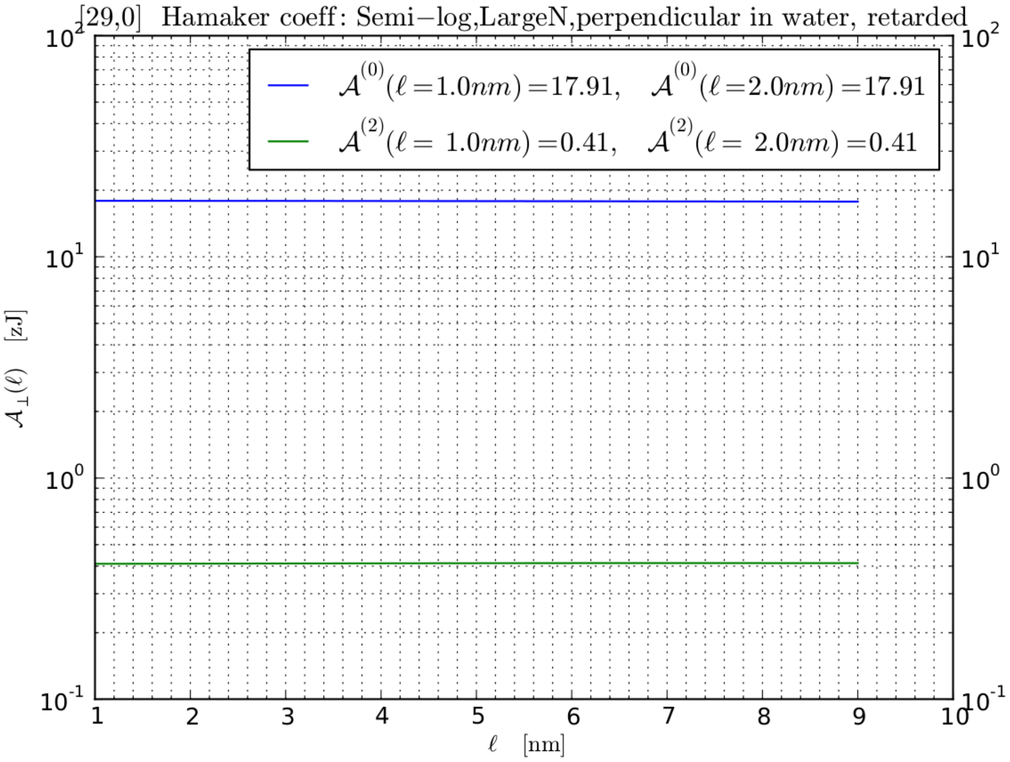


Figure 20: Full result

$$\mathcal{A}^{(2)}(\ell) = \frac{k_BT}{32}{\sum_{n=0}^{\infty}}' \Delta_{1,\|}\Delta_{2,\|}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{57}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{58}$$

Knee in plots of $\mathcal{A}^{(0)}$ as a function of separation

10 An example plot of knee: $\mathcal{A}^{(0)}$ for [9,3]

$$\mathcal{A}^{(0)}(\ell) = \frac{k_BT}{32}{\sum_{n=0}^{\infty}}' \Delta_{1,\|}\Delta_{2,\|}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{59}$$

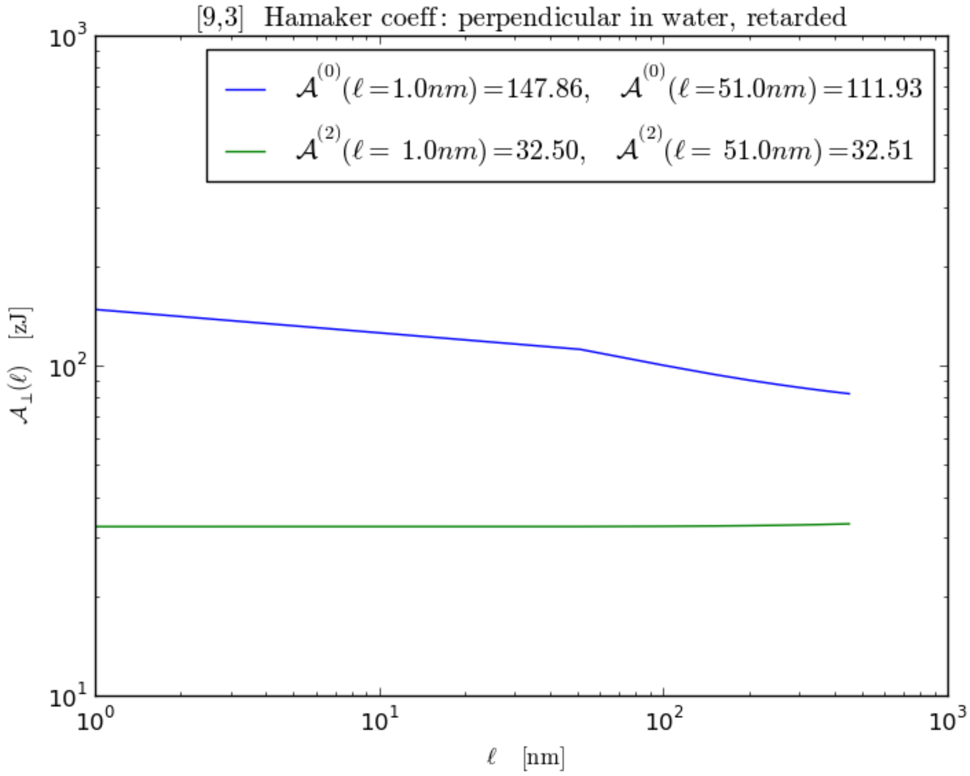


Figure 21: $\mathcal{A}^{(0)}$ as a function of separation appears to have a knee near 36 nm.

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) = \\ 2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right]$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_BT}{32}{\sum_{n=0}^{\infty}}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{60}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{61}$$

The (ℓ) dependence of the Hamaker coefficients $\mathcal{A}$ is a consequence of (ℓ) dependence of $p_n^2(\ell) = \epsilon_m(i\omega_n)\frac{\omega_n^2}{c^2}\ell^2$

$$\mathcal{A}^{(0)}(\ell) = \frac{k_B T}{32} {\sum_{n=0}^{\infty}}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{62}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) = 2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right] \tag{63}$$

and

$$\mathcal{A}^{(2)}(\ell) = \frac{k_B T}{32} {\sum_{n=0}^{\infty}}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{64}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{65}$$

$\zeta_n = 2\pi n k_B T/\hbar$, where n is an integer and the $n = 0$ term is counted with a weight 1/2.
where $p_n^2(\ell) = \epsilon_m(i\omega_n)\frac{\omega_n^2}{c^2}\ell^2$.

11 Plots of how each Matsubara term contributes to $\mathcal{A}_n^{(0)}(\ell)$

11.1 Plots for visualizing and comparing gradiants for different CNT's

Surface plots for Hamaker Coefficients as function of angle and separation

12 Fully Retarded

12.1 $\mathcal{A}^{(0)}$ for [6,5], [9,1], and [29,0] in water

$$\mathcal{A}^{(0)}(\ell) = \frac{k_B T}{32} {\sum_{n=0}^{\infty}}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{66}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) = 2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right] \tag{67}$$

and

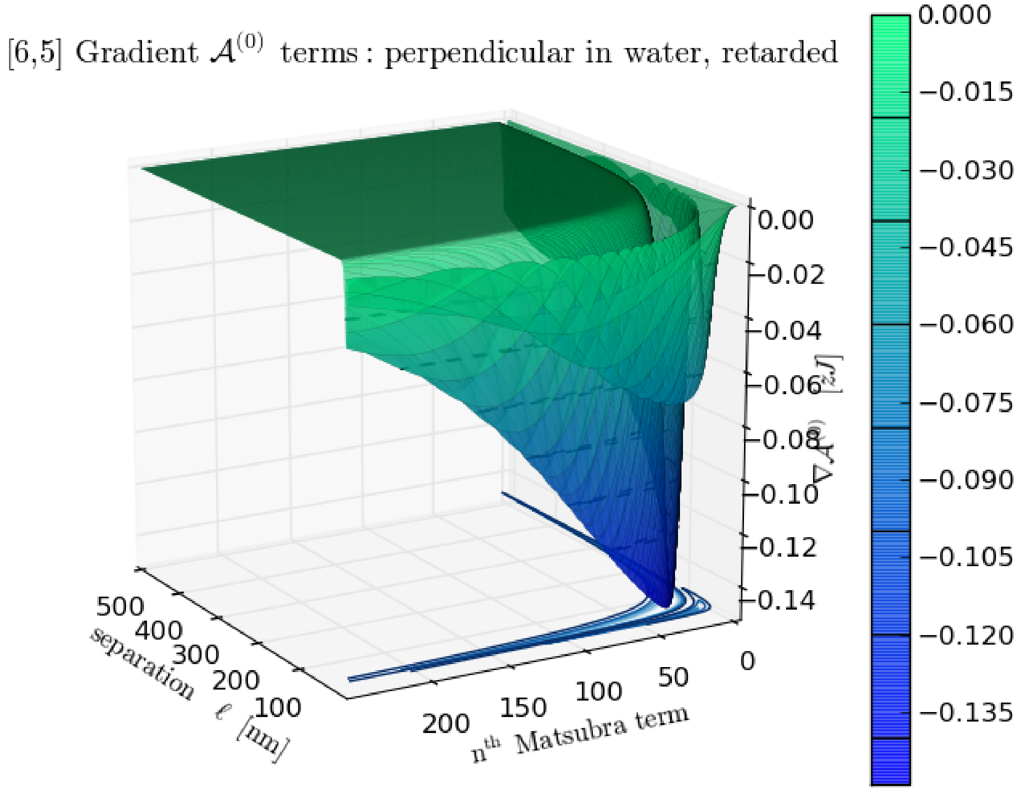


Figure 22: $\nabla(\mathcal{A}_n^{(0)}(\ell))$ for [6,5]: derivative of $\mathcal{A}_n^{(0)}(\ell)$ (z-axis) with respect to separation and n (x and y axes. $Max[|\nabla(\mathcal{A}^{(0)})|]$ occurs at $\ell = \ell_{knee}$

$$\mathcal{A}^{(2)}(\ell) = \frac{k_B T}{32} \sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{68}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{69}$$

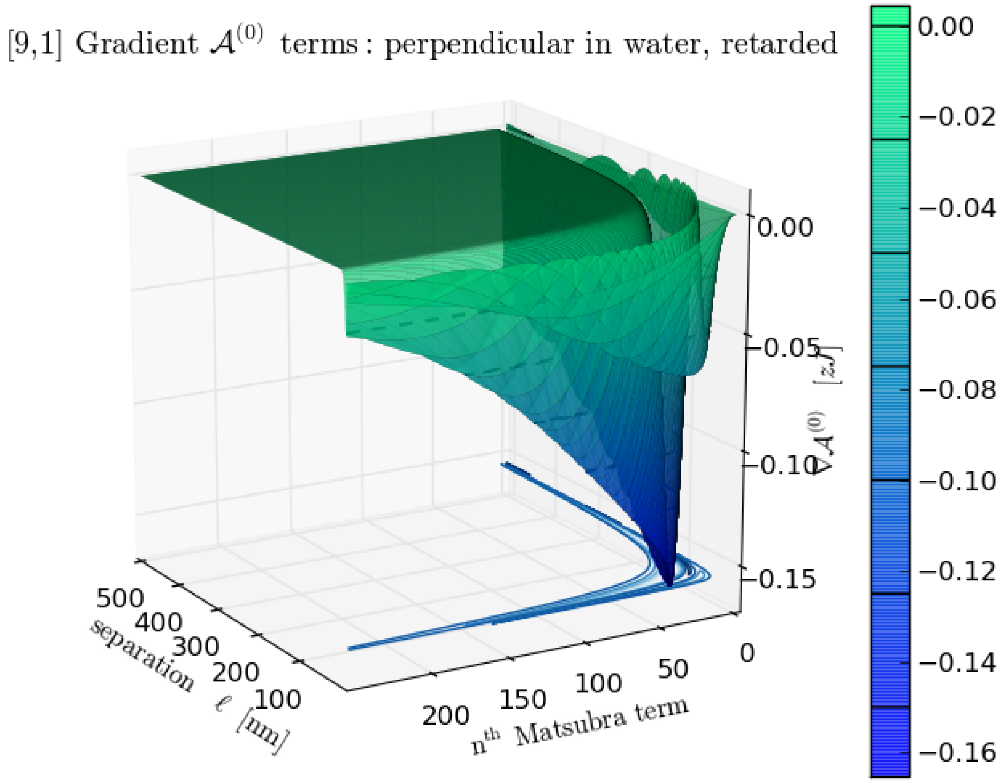


Figure 23: $\nabla(\mathcal{A}_n^{(0)}(\ell))$ for [9,1]: derivative of $\mathcal{A}_n^{(0)}(\ell)$ (z-axis) with respect to separation and n (x and y axes. $Max[|\nabla(\mathcal{A}^{(0)})|]$ occurs at $\ell = \ell_{knee}$

12.2 Hamaker 2: $\mathcal{A}^{(2)}$ for [6,5], [9,1], and [29,0] in water

$$\mathcal{A}^{(0)}(\ell) = \frac{k_B T}{32} \sum_{n=0}^{\infty}{}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell) \int_0^\infty tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{70}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) = 2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right] \tag{71}$$

and

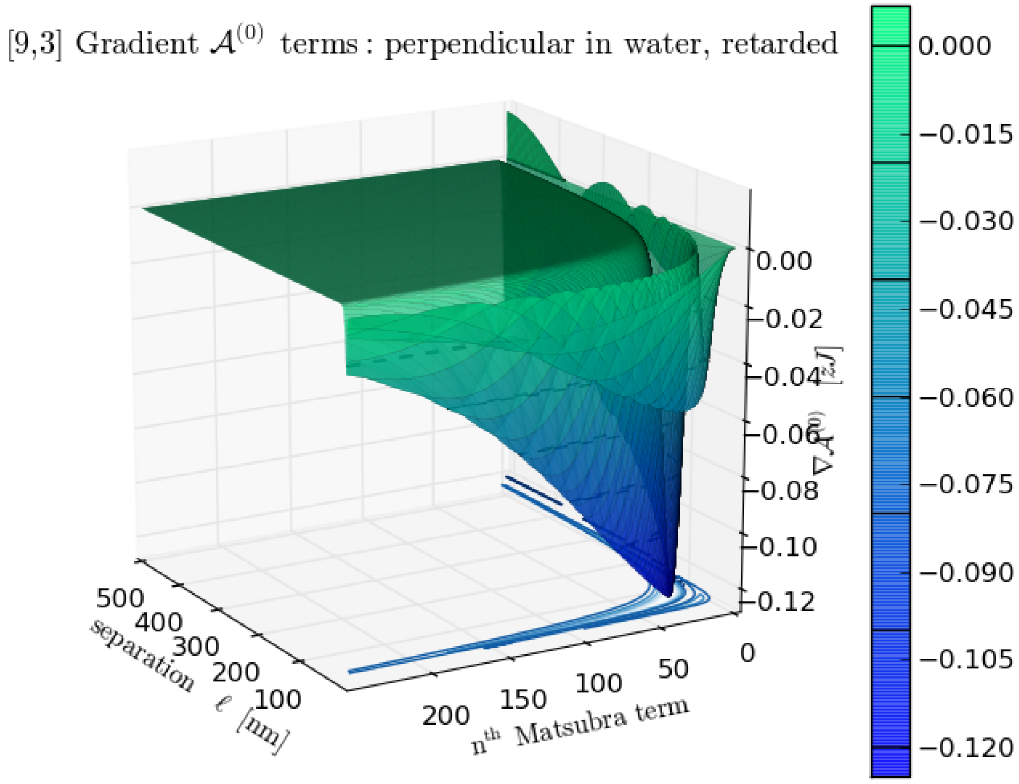


Figure 24: $\nabla(\mathcal{A}_n^{(0)}(\ell))$ for [9,3]: derivative of $\mathcal{A}_n^{(0)}(\ell)$ (z-axis) with respect to separation and n (x and y axes. $Max[|\nabla(\mathcal{A}^{(0)})|]$ occurs at $\ell = \ell_{knee}$

$$\mathcal{A}^{(2)}(\ell) = \frac{k_B T}{32} \sum_{n=0}^{\infty}{}' \Delta_{1,\|}\Delta_{2,\|}\, p_n^4(\ell) \int_0^\infty t dt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)} \tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{72}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{73}$$

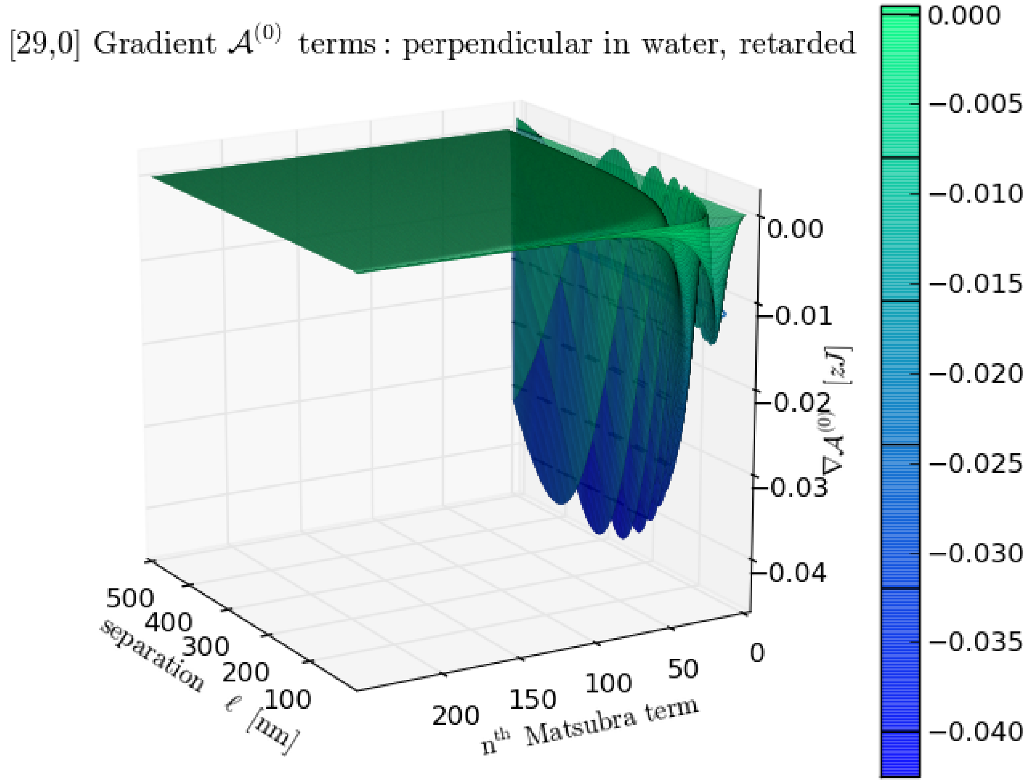


Figure 25: $\nabla(\mathcal{A}_n^{(0)}(\ell))$ for [29,0]: derivative of $\mathcal{A}_n^{(0)}(\ell)$ (z-axis) with respect to separation and n (x and y axes. $Max[|\nabla(\mathcal{A}^{(0)})|]$ occurs at $\ell = \ell_{knee}$

12.3 Total Hamaker: $\mathcal{A} = \mathcal{A}^{(0)} + \mathcal{A}^{(2)}$ for [6,5], [9,1], and [29,0] in water

$$\mathcal{A}^{(0)}(\ell) = \frac{k_BT}{32}\sum_{n=0}^{\infty}{}' \Delta_{1,\|}\Delta_{2,\|}\, p_n^4(\ell) \int_0^\infty tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)}\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) \tag{74}$$

with

$$\tilde{g}^{(0)}(t, a_1(i\omega_n), a_2(i\omega_n)) = 2\left[(1+3a_1)(1+3a_2)t^4 + 2(1+2a_1+2a_2+3a_1a_2)t^2 + 2(1+a_1)(1+a_2)\right] \tag{75}$$

and

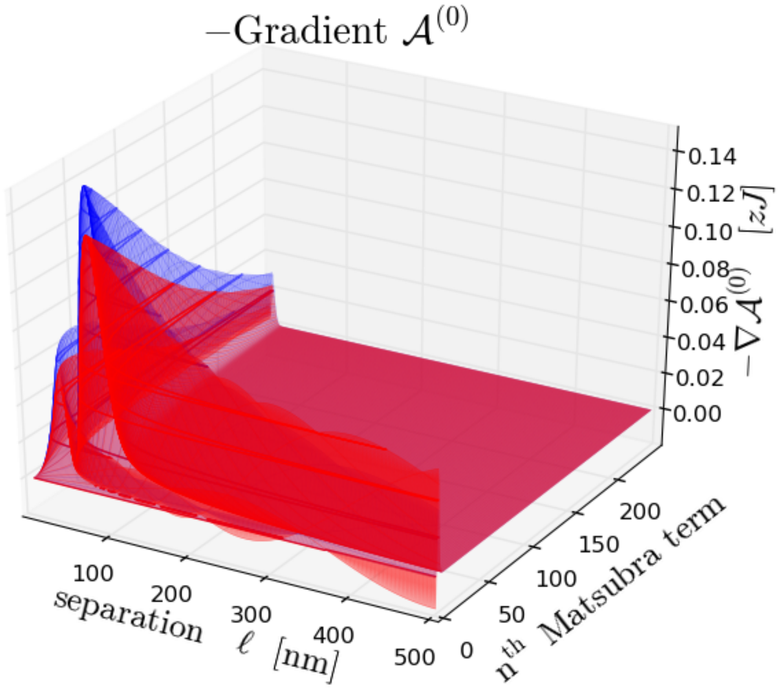


Figure 26: $-\nabla(\mathcal{A}_n^{(0)}(\ell))$ for [6,5] (blue) and [9,3] (red)

$$\mathcal{A}^{(2)}(\ell) = \frac{k_BT}{32}{\sum_{n=0}^{\infty}}' \Delta_{1,\parallel}\Delta_{2,\parallel}\, p_n^4(\ell)\, \int_0^{\infty} tdt\, \frac{e^{-2p_n(\ell)\sqrt{t^2+1}}}{(t^2+1)}\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) \tag{76}$$

with

$$\tilde{g}^{(2)}(t, a_1(i\omega_n), a_2(i\omega_n), \theta) = (1-a_1)(1-a_2)(t^2+2)^2 \tag{77}$$

Tables

13 Table of published results

14 Table of python results

*data from Chirality-dependent properties of carbon nanotubes: electronic structure, optical dispersion properties, Hamaker coefficients and van der

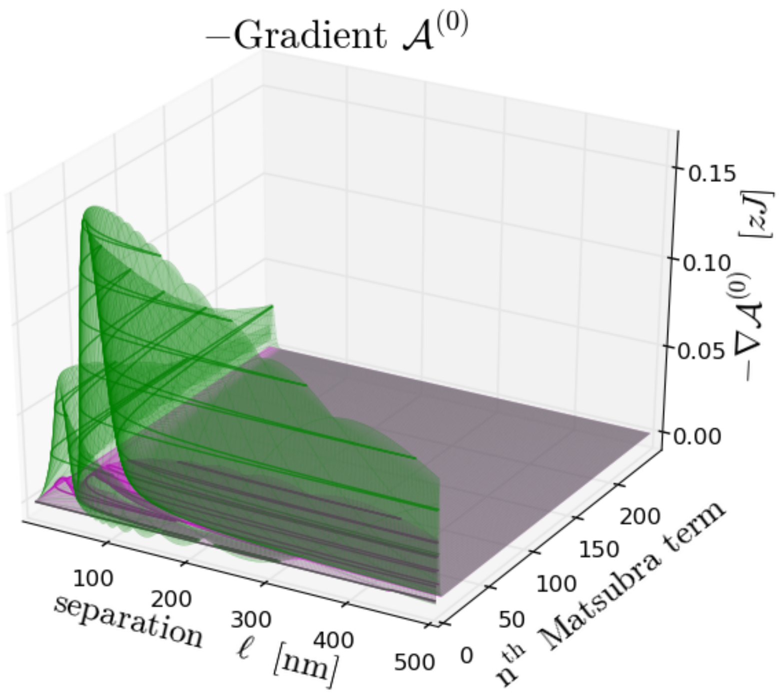


Figure 27: $-\nabla(\mathcal{A}_n^{(0)}(\ell))$ for [9,1] (green) and [29,0] (magenta)

WaalsLondon dispersion interactions Rick F. Rajter, Roger H. French, W.Y. Ching, Rudolf Podgornik and V. Adrian Parsegian RSC Adv., 2013,3, 823-842 DOI: 10.1039/C2RA20083J

15 Table of Gecko Hamaker results

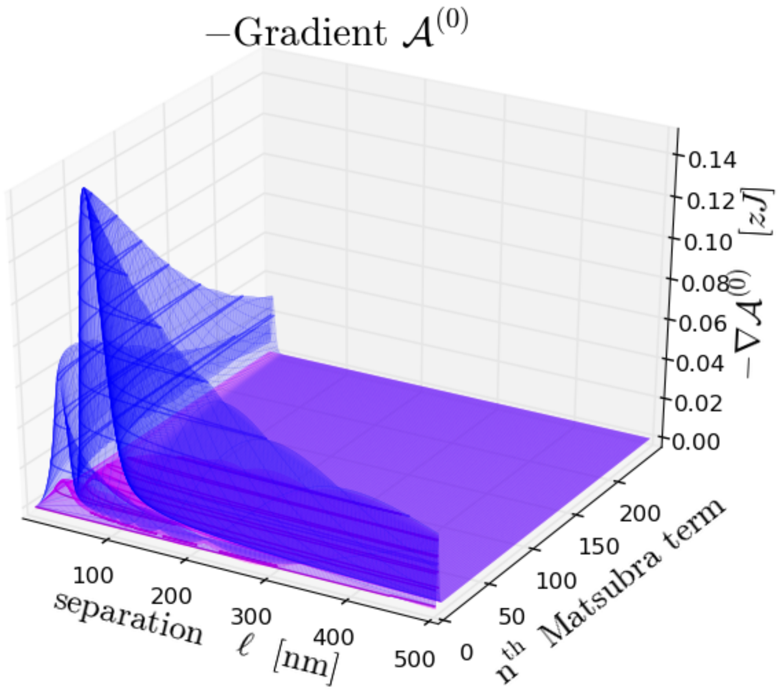


Figure 28: $-\nabla(\mathcal{A}_n^{(0)}(\ell))$ for [6,5] (blue) and [29,0] (magenta)

Table 1: Rajter results from IJMR perpendiuclar cylinders in water (Rajter's spectrum)

CNT	$\mathcal{A}^0$ [zJ]	$\mathcal{A}^2$ [zJ]
[6,5]	106	1.9
[9,0]	-	
[9,1]	92.8	3
[9,3]	107	36.2
[29,0]	18.5	0.8

Table 2: Python results, retarded formulation: perpendiuclar cylinders in water, intersurface distance = 1 nm

CNT	atoms*	radius*[A]	Type*	Geom*	$\mathcal{A}^0$(n=0) [zJ]	$\mathcal{A}^0$ [zJ]	$\mathcal{A}^2$ [zJ]
[6,5]	364	3.734	sc	chiral	1x5.46	105.46	0.96
[9,0]			semi-metal; in progress				
[9,1]	364	3.734	sc	chiral	1x5.46	93.56	1.56
[9,3]	156	4.234	sm	chiral	1x5.46	83.06	3.23
[29,0]	116	11.352	sc	zigzag	1x5.46	17.73	0.41

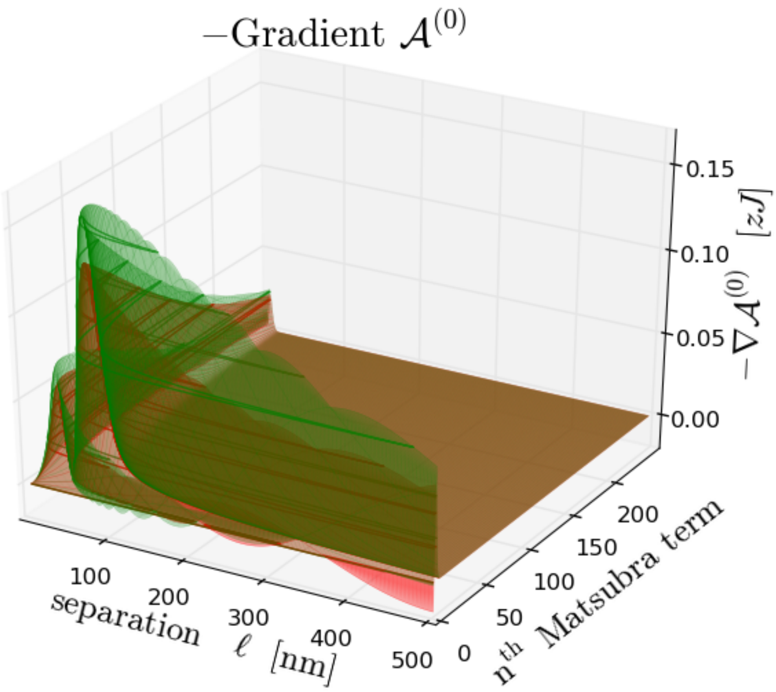


Figure 29: $-\nabla(\mathcal{A}_n^{(0)}(\ell))$ for [9,1] (red) and [9,3] (green)

Table 3: Python results, non-retarded formulation: perpendiuclar cylinders in water

CNT	$\mathcal{A}^0$ [zJ]	$\mathcal{A}^2$ [zJ]
[6,5]	126.80	1.16
[9,0]	semi-metal; in progress	
[9,1]	112.22	1.87
[9,3]	semi-metal; in progress	
[29,0]	20.93	0.49

Table 4: Gecko Hamaker results from 2.07, perpendiuclar cylinders in water

CNT	$\mathcal{A}^0$ [zJ]	$\mathcal{A}^2$ [zJ]
[6,5]	100	1.04
[9,0]	151	6.96
[9,1]	84.85	1.16
[9,3]	80.66	1.55
[29,0]	17.68	0.22

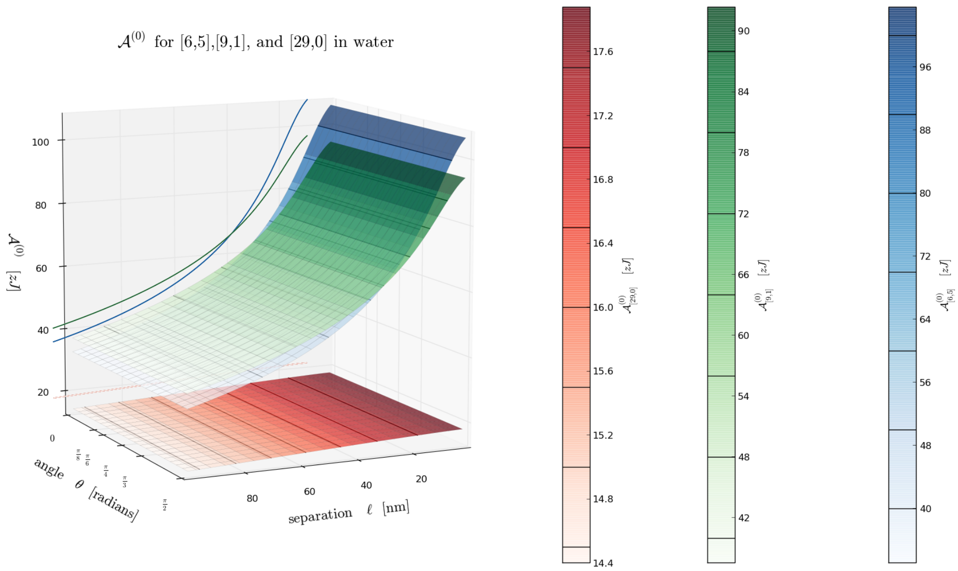


Figure 30: $\mathcal{A}^{(0)}$ for [6,5], [9,1], and [29,0] in water. No theta dependence

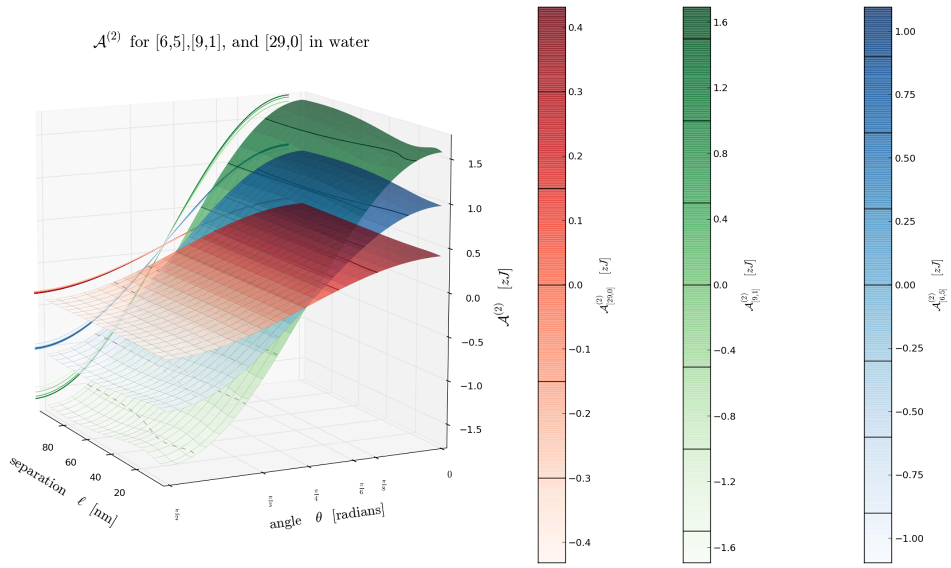


Figure 31: $\mathcal{A}^{(2)}$ for [6,5], [9,1], and [29,0] in water.

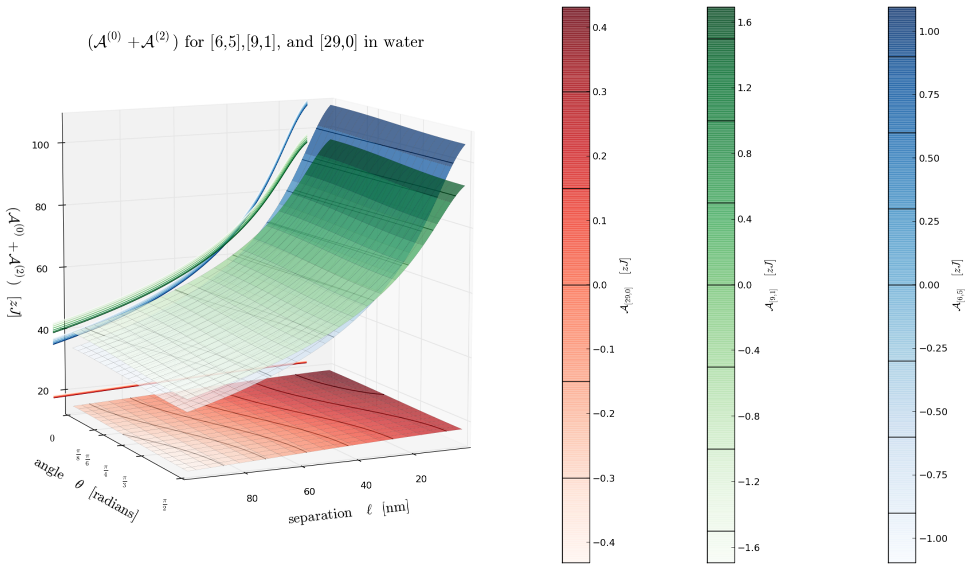


Figure 32: $\mathcal{A} = \mathcal{A}^{(0)} + \mathcal{A}^{(2)}$ for [6,5], [9,1], and [29,0] in water