Coupled dynamics in binary mixtures of colloidal Yukawa systems

Daniel Weidig and Joachim Wagner[a)]
Institut für Chemie, Universität Rostock, 18051 Rostock, Germany

Compilation of the numerical values for the reduced long-time self-diffusion coefficient $D_{S,\alpha}^{(L),\mathrm{red}}$ and stretched exponential parameters, relaxation rates $a_{\alpha\beta}$ and stretching exponent $b_{\alpha\beta}$, of binary Yukawa-suspensions of identically charged but differently sized species.

I. NUMERICAL DATA

TABLE I. Reduced long-time self-diffusion coefficient $D_{S}^{(L),\mathrm{red}}$ of one-component Yukawa-suspensions in dependence on the particle diameter σ and number of effective charges Z_{eff} at number density ${}^{1}\rho = 1 \times 10^{18}\,\mathrm{m}^{-3}$.

Z_{eff}	$\sigma = 100\,\mathrm{nm}$	$\sigma = 50\,\mathrm{nm}$	$\sigma = 33\,\mathrm{nm}$	$\sigma = 25\,\mathrm{nm}$	$\sigma = 20\,\mathrm{nm}$
300	0.2771 (24)	0.2765 (22)	0.2757 (25)	0.2749 (21)	0.2761 (22)
350	0.2193 (26)	0.2172 (20)	0.2171 (17)	0.2176 (18)	0.2175 (18)
400	0.1689 (23)	0.1687 (20)	0.1686 (22)	0.1678 (19)	0.1680 (15)
450	0.1308 (21)	0.1277 (15)	0.1272 (15)	0.1264 (12)	0.1267 (12)
500	0.0907 (28)	0.0918 (18)	0.0919 (17)	0.0919 (22)	0.0909 (22)
550	0.0638 (20)	0.0645 (23)	0.0650 (18)	0.0639 (16)	0.0640 (27)
600	0.0432 (14)	0.0435 (20)	0.0428 (11)	0.0422 (17)	0.0415 (20)

a) Electronic mail: joachim.wagner@uni-rostock.de

TABLE II. Reduced long-time self-diffusion coefficients $D_{\mathrm{S},\alpha}^{(\mathrm{L}),\mathrm{red}}$ of binary colloidal suspensions in dependence on their number of effective charges Z_{eff}, their diameter ratio $\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}}$ and their number density ratio ${}^1\rho_{\mathrm{B}}/{}^1\rho_{\mathrm{A}}$. The larger species A has the diameter $\sigma_{\mathrm{A}} = 100\,\mathrm{nm}$ and total number density is ${}^1\rho_{\mathrm{tot}} = 1\times10^{18}\,\mathrm{m}^{-3}$.

${}^1\rho_{\mathrm{B}}/{}^1\rho_{\mathrm{A}}$	Z_{eff}	$\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}}=2$		$\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}}=3$		$\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}}=4$		$\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}}=5$	
		$D_{\mathrm{S,A}}^{(\mathrm{L}),\mathrm{red}}$	$D_{\mathrm{S,B}}^{(\mathrm{L}),\mathrm{red}}$	$D_{\mathrm{S,A}}^{(\mathrm{L}),\mathrm{red}}$	$D_{\mathrm{S,B}}^{(\mathrm{L}),\mathrm{red}}$	$D_{\mathrm{S,A}}^{(\mathrm{L}),\mathrm{red}}$	$D_{\mathrm{S,B}}^{(\mathrm{L}),\mathrm{red}}$	$D_{\mathrm{S,A}}^{(\mathrm{L}),\mathrm{red}}$	$D_{\mathrm{S,B}}^{(\mathrm{L}),\mathrm{red}}$
1	300	0.338 (6)	0.216 (3)	0.380 (8)	0.182 (3)	0.397 (5)	0.1633 (18)	0.419 (5)	0.1485 (20)
	350	0.273 (5)	0.1665 (22)	0.303 (7)	0.137 (4)	0.324 (6)	0.1214 (20)	0.342 (5)	0.1100 (18)
	400	0.213 (4)	0.126 (3)	0.240 (4)	0.1035 (25)	0.256 (5)	0.0886 (20)	0.2683 (20)	0.0793 (15)
	450	0.167 (4)	0.0952 (19)	0.185 (4)	0.0749 (22)	0.195 (4)	0.0641 (16)	0.209 (5)	0.0569 (15)
	500	0.119 (4)	0.0658 (21)	0.133 (4)	0.0522 (16)	0.144 (4)	0.0445 (12)	0.1511 (29)	0.0382 (14)
	550	0.0827 (25)	0.0446 (12)	0.0948 (27)	0.0358 (10)	0.101 (5)	0.0301 (18)	0.1067 (22)	0.0257 (8)
	600	0.0554 (29)	0.0298 (17)	0.0640 (27)	0.0232 (12)	0.0681 (28)	0.0193 (10)	0.0700 (29)	0.0161 (7)
2	300	0.365 (6)	0.233 (4)	0.417 (7)	0.209 (4)	0.451 (7)	0.1941 (23)	0.478 (8)	0.183 (3)
	350	0.296 (6)	0.182 (4)	0.343 (6)	0.1615 (23)	0.372 (7)	0.1468 (25)	0.399 (6)	0.1367 (21)
	400	0.234 (6)	0.139 (3)	0.273 (5)	0.1203 (27)	0.298 (3)	0.1082 (22)	0.325 (6)	0.1018 (18)
	450	0.181 (5)	0.1040 (18)	0.214 (5)	0.0895 (26)	0.231 (3)	0.0789 (13)	0.253 (7)	0.0729 (13)
	500	0.130 (4)	0.0727 (25)	0.154 (5)	0.0626 (15)	0.174 (6)	0.0554 (15)	0.188 (7)	0.0504 (19)
	550	0.092 (4)	0.0508 (16)	0.112 (4)	0.0433 (17)	0.125 (6)	0.0380 (13)	0.135 (5)	0.0337 (10)
	600	0.063 (4)	0.0337 (18)	0.074 (4)	0.0278 (10)	0.083 (3)	0.0237 (12)	0.090 (4)	0.0215 (5)
4	300	0.385 (10)	0.250 (4)	0.458 (9)	0.2341 (22)	0.492 (10)	0.2235 (25)	0.537 (12)	0.2168 (26)
	350	0.314 (8)	0.195 (4)	0.379 (7)	0.1814 (21)	0.417 (7)	0.1726 (23)	0.454 (8)	0.1658 (20)
	400	0.250 (7)	0.150 (3)	0.305 (9)	0.1386 (23)	0.340 (7)	0.1290 (21)	0.373 (11)	0.1231 (21)
	450	0.193 (5)	0.1127 (16)	0.236 (8)	0.1022 (25)	0.267 (10)	0.0946 (17)	0.297 (7)	0.0909 (20)
	500	0.142 (4)	0.0802 (21)	0.178 (6)	0.0732 (18)	0.202 (6)	0.0674 (18)	0.225 (6)	0.0633 (17)
	550	0.101 (5)	0.0563 (22)	0.129 (6)	0.0495 (13)	0.148 (7)	0.0460 (18)	0.162 (6)	0.0429 (15)
	600	0.067 (4)	0.0361 (15)	0.085 (6)	0.0320 (21)	0.098 (5)	0.0292 (15)	0.110 (6)	0.0274 (15)

TABLE III. Exponential decay constant a and stretching exponent b of a virtually binary mixture in dependence on the particle diameter σ and its number of effective charges Z_{eff} at identical number densities ${}^1\rho_{\mathrm{A}} = {}^1\rho_{\mathrm{B}} = 5\times10^{17}\,\mathrm{m}^{-3}$.

Z_{eff}	$\sigma = 100\,\mathrm{nm}$		$\sigma = 50\,\mathrm{nm}$		$\sigma = 33\,\mathrm{nm}$		$\sigma = 25\,\mathrm{nm}$	
	a / ms^{-1}	b	a / ms^{-1}	b	a / ms^{-1}	b	a / ms^{-1}	b
300	0.0404 (5)	1.108 (10)	0.0822 (11)	1.115 (7)	0.1245 (9)	1.112 (6)	0.1635 (18)	1.112 (5)
350	0.0320 (4)	1.043 (6)	0.0642 (6)	1.043 (4)	0.0980 (8)	1.047 (4)	0.1284 (10)	1.044 (4)
400	0.0243 (5)	0.978 (7)	0.0489 (4)	0.9791 (26)	0.0741 (7)	0.981 (5)	0.0988 (29)	0.978 (18)
450	0.01786 (23)	0.920 (5)	0.0362 (6)	0.920 (7)	0.0549 (4)	0.920 (4)	0.0729 (6)	0.923 (22)
500	0.01262 (28)	0.864 (8)	0.0255 (5)	0.862 (4)	0.0395 (5)	0.869 (4)	0.0518 (4)	0.867 (4)
550	0.0085 (3)	0.807 (14)	0.0173 (5)	0.811 (7)	0.0261 (4)	0.810 (5)	0.0348 (4)	0.8095 (27)
600	0.00508 (15)	0.746 (10)	0.0109 (4)	0.756 (8)	0.01651 (21)	0.754 (5)	0.0216 (5)	0.754 (5)

TABLE IV. Exponential decay constant a and stretching exponent b of binary Yukawa-suspensions of identical charged but differently sized colloidal particles in dependence on the number of effective charges Z_{eff} and the ratio of the species diameters $\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}}$ for a ratio of the number densities ${}^{1}\rho_{\mathrm{B}}/{}^{1}\rho_{\mathrm{A}} = 1$. The total number density for all suspensions is identical ${}^{1}\rho_{\mathrm{tot}} = 1 \times 10^{18}\,\mathrm{m}^{-3}$, the diameter of species A is constant $\sigma_{\mathrm{A}} = 100\,\mathrm{nm}$.

${}^{1}\rho_{\mathrm{B}}/{}^{1}\rho_{\mathrm{A}}$	Z_{eff}	$\alpha\beta$	$\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}} = 2$ AA	AB	BB	$\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}} = 3$ AA	AB	BB	$\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}} = 4$ AA	AB	BB
1	300	$a_{\alpha\beta}$	0.0472 (13)	0.0554 (8)	0.0662 (8)	0.0515 (13)	0.0644 (13)	0.0873 (13)	0.0535 (12)	0.0707 (14)	0.1046 (21)
		$b_{\alpha\beta}$	1.177 (18)	1.094 (11)	1.013 (13)	1.211 (15)	1.085 (11)	0.958 (6)	1.224 (12)	1.076 (6)	0.918 (8)
	350	$a_{\alpha\beta}$	0.0385 (7)	0.0433 (5)	0.0502 (9)	0.0423 (8)	0.0510 (7)	0.0647 (9)	0.0441 (9)	0.0555 (7)	0.0752 (12)
		$b_{\alpha\beta}$	1.101 (10)	1.032 (6)	0.960 (9)	1.136 (11)	1.028 (10)	0.911 (9)	1.153 (13)	1.023 (6)	0.879 (10)
	400	$a_{\alpha\beta}$	0.0297 (6)	0.0332 (5)	0.0367 (10)	0.0335 (8)	0.0387 (7)	0.0464 (9)	0.0355 (10)	0.0423 (8)	0.0536 (10)
		$b_{\alpha\beta}$	1.030 (10)	0.970 (7)	0.911 (12)	1.066 (9)	0.973 (6)	0.871 (6)	1.086 (11)	0.971 (5)	0.847 (8)
	450	$a_{\alpha\beta}$	0.0225 (6)	0.0243 (10)	0.0264 (5)	0.0255 (6)	0.0285 (6)	0.0328 (8)	0.0270 (7)	0.0311 (6)	0.0369 (6)
		$b_{\alpha\beta}$	0.966 (7)	0.918 (10)	0.867 (8)	0.998 (14)	0.918 (8)	0.833 (8)	1.007 (7)	0.915 (9)	0.811 (6)
	500	$a_{\alpha\beta}$	0.0166 (5)	0.0174 (4)	0.0184 (4)	0.0185 (4)	0.0202 (4)	0.0221 (5)	0.0196 (6)	0.0218 (6)	0.0248 (6)
		$b_{\alpha\beta}$	0.910 (10)	0.866 (9)	0.823 (9)	0.924 (8)	0.864 (7)	0.798 (5)	0.933 (13)	0.862 (11)	0.782 (8)
	550	$a_{\alpha\beta}$	0.0111 (4)	0.0116 (5)	0.0121 (5)	0.01258 (28)	0.01338 (28)	0.0144 (4)	0.0137 (3)	0.01468 (29)	0.0161 (5)
		$b_{\alpha\beta}$	0.838 (10)	0.811 (10)	0.780 (10)	0.855 (9)	0.809 (7)	0.758 (10)	0.865 (8)	0.809 (8)	0.751 (10)
	600	$a_{\alpha\beta}$	0.0070 (4)	0.0072 (3)	0.0074 (4)	0.0079 (4)	0.0082 (5)	0.0086 (6)	0.00863 (26)	0.0090 (4)	0.0094 (4)
		$b_{\alpha\beta}$	0.773 (17)	0.750 (15)	0.728 (15)	0.785 (14)	0.751 (16)	0.714 (19)	0.795 (9)	0.755 (9)	0.711 (11)

TABLE V. Exponential decay constant a and stretching exponent b of binary Yukawa-suspensions of identical charged but differently sized colloidal particles in dependence on the number of effective charges Z_{eff} and the ratio of the species diameters $\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}}$ for a ratio of the number densities ${}^{1}\rho_{\mathrm{B}}/{}^{1}\rho_{\mathrm{A}} = 2$. The total number density for all suspensions is identical ${}^{1}\rho_{\mathrm{tot}} = 1 \times 10^{18}\,\mathrm{m}^{-3}$, the diameter of species A is constant $\sigma_{\mathrm{A}} = 100\,\mathrm{nm}$.

${}^{1}\rho_{\mathrm{B}}/{}^{1}\rho_{\mathrm{A}}$	Z_{eff}		$\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}} = 2$			$\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}} = 3$			$\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}} = 4$		
		$\alpha\beta$	AA	AB	BB	AA	AB	BB	AA	AB	BB
2	300	$a_{\alpha\beta}$	0.0504 (18)	0.0588 (10)	0.0709 (13)	0.0559 (16)	0.0709 (14)	0.0979 (14)	0.0594 (11)	0.0787 (14)	0.1210 (16)
		$b_{\alpha\beta}$	1.196 (19)	1.117 (9)	1.038 (11)	1.251 (22)	1.122 (11)	0.991 (4)	1.268 (20)	1.114 (11)	0.954 (8)
	350	$a_{\alpha\beta}$	0.0409 (7)	0.0466 (9)	0.0541 (11)	0.0465 (10)	0.0566 (11)	0.0733 (11)	0.0498 (12)	0.0639 (9)	0.0901 (8)
		$b_{\alpha\beta}$	1.128 (11)	1.059 (10)	0.981 (9)	1.175 (17)	1.064 (11)	0.946 (7)	1.201 (10)	1.062 (8)	0.918 (8)
	400	$a_{\alpha\beta}$	0.0330 (10)	0.0363 (9)	0.0407 (6)	0.0376 (9)	0.0442 (8)	0.0543 (7)	0.0402 (9)	0.0496 (9)	0.0653 (8)
		$b_{\alpha\beta}$	1.070 (16)	0.999 (10)	0.931 (6)	1.105 (12)	1.010 (6)	0.903 (7)	1.126 (13)	1.007 (7)	0.879 (5)
	450	$a_{\alpha\beta}$	0.0246 (10)	0.0267 (15)	0.0292 (11)	0.0289 (9)	0.0328 (7)	0.0388 (8)	0.0320 (10)	0.0375 (6)	0.0458 (8)
		$b_{\alpha\beta}$	0.992 (17)	0.938 (14)	0.882 (11)	1.028 (13)	0.945 (10)	0.861 (6)	1.056 (14)	0.955 (4)	0.841 (7)
	500	$a_{\alpha\beta}$	0.0181 (6)	0.0191 (4)	0.0205 (5)	0.0213 (6)	0.0237 (7)	0.0265 (7)	0.0236 (4)	0.02676 (24)	0.0311 (6)
		$b_{\alpha\beta}$	0.929 (9)	0.881 (5)	0.837 (8)	0.953 (9)	0.890 (8)	0.817 (8)	0.979 (8)	0.897 (7)	0.804 (9)
	550	$a_{\alpha\beta}$	0.0123 (4)	0.0128 (4)	0.0134 (5)	0.0149 (6)	0.0161 (6)	0.0174 (8)	0.0165 (5)	0.01802 (26)	0.0201 (5)
		$b_{\alpha\beta}$	0.853 (11)	0.821 (6)	0.786 (8)	0.884 (11)	0.833 (10)	0.777 (12)	0.899 (11)	0.834 (5)	0.765 (6)
	600	$a_{\alpha\beta}$	0.00774 (24)	0.00787 (27)	0.00807 (25)	0.0095 (5)	0.0099 (5)	0.0104 (5)	0.0105 (4)	0.0113 (4)	0.0121 (5)
		$b_{\alpha\beta}$	0.785 (17)	0.756 (10)	0.733 (9)	0.809 (15)	0.770 (13)	0.727 (12)	0.818 (12)	0.772 (7)	0.722 (9)

TABLE VI. Exponential decay constant a and stretching exponent b of binary Yukawa-suspensions of identical charged but differently sized colloidal particles in dependence on the number of effective charges Z_{eff} and the ratio of the species diameters $\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}}$ for a ratio of the number densities ${}^{1}\rho_{\mathrm{B}}/{}^{1}\rho_{\mathrm{A}} = 4$. The total number density for all suspensions is identical ${}^{1}\rho_{\mathrm{tot}} = 1 \times 10^{18}\,\mathrm{m}^{-3}$, the diameter of species A is constant $\sigma_{\mathrm{A}} = 100\,\mathrm{nm}$.

${}^{1}\rho_{\mathrm{B}}/{}^{1}\rho_{\mathrm{A}}$	Z_{eff}		$\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}} = 2$			$\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}} = 3$			$\sigma_{\mathrm{A}}/\sigma_{\mathrm{B}} = 4$		
		$\alpha\beta$	AA	AB	BB	AA	AB	BB	AA	AB	BB
4	300	$a_{\alpha\beta}$	0.0520 (27)	0.0615 (14)	0.0748 (12)	0.0592 (18)	0.0760 (18)	0.1072 (17)	0.0637 (28)	0.0862 (11)	0.1362 (11)
		$b_{\alpha\beta}$	1.22 (4)	1.139 (10)	1.057 (9)	1.26 (29)	1.150 (13)	1.024 (8)	1.31 (5)	1.154 (9)	0.999 (7)
	350	$a_{\alpha\beta}$	0.0429 (14)	0.0489 (8)	0.0576 (8)	0.0500 (7)	0.0617 (8)	0.0818 (9)	0.0542 (15)	0.0706 (10)	0.1034 (9)
		$b_{\alpha\beta}$	1.146 (15)	1.073 (9)	1.000 (7)	1.217 (28)	1.094 (9)	0.974 (7)	1.244 (22)	1.099 (9)	0.957 (5)
	400	$a_{\alpha\beta}$	0.0345 (13)	0.0384 (7)	0.0436 (7)	0.0405 (15)	0.0488 (6)	0.0612 (8)	0.0450 (13)	0.0561 (10)	0.0765 (14)
		$b_{\alpha\beta}$	1.077 (19)	1.012 (10)	0.949 (6)	1.126 (19)	1.035 (7)	0.928 (4)	1.171 (19)	1.045 (8)	0.911 (6)
	450	$a_{\alpha\beta}$	0.0263 (10)	0.0287 (13)	0.0318 (9)	0.0318 (10)	0.0376 (7)	0.0448 (7)	0.0364 (11)	0.0433 (8)	0.0551 (11)
		$b_{\alpha\beta}$	1.013 (20)	0.953 (12)	0.897 (6)	1.058 (17)	0.978 (10)	0.884 (5)	1.098 (18)	0.988 (8)	0.871 (6)
	500	$a_{\alpha\beta}$	0.0195 (8)	0.0210 (6)	0.0225 (6)	0.0242 (7)	0.0271 (7)	0.0308 (6)	0.0275 (13)	0.0318 (9)	0.0380 (7)
		$b_{\alpha\beta}$	0.941 (14)	0.898 (10)	0.849 (7)	0.986 (14)	0.915 (9)	0.835 (6)	1.017 (22)	0.927 (10)	0.828 (4)
	550	$a_{\alpha\beta}$	0.0134 (6)	0.0141 (4)	0.0149 (4)	0.0174 (8)	0.0185 (6)	0.0203 (6)	0.0195 (7)	0.0221 (5)	0.0250 (6)
		$b_{\alpha\beta}$	0.872 (12)	0.834 (10)	0.798 (7)	0.914 (21)	0.850 (9)	0.788 (8)	0.935 (15)	0.864 (6)	0.787 (9)
	600	$a_{\alpha\beta}$	0.0084 (4)	0.0089 (4)	0.0092 (4)	0.0112 (6)	0.0118 (4)	0.01253 (28)	0.0130 (5)	0.0139 (6)	0.0152 (8)
		$b_{\alpha\beta}$	0.788 (24)	0.770 (15)	0.744 (12)	0.834 (18)	0.790 (7)	0.741 (6)	0.847 (14)	0.796 (12)	0.738 (13)

TABLE VII. Coupling constant ζ in dependence on the number of effective charges Z_{eff}.

Z_{eff}	300	350	400	450	500	550	600
$\zeta \times 10^2$	1.28_2	1.092_{14}	0.941_{13}	0.737_{11}	0.555_9	0.391_8	0.249_7