Excluded-volume short-range repulsive potential for tetrahedral molecules

F. Bisi[a], G. Pająk[b], L. Longa[b], R. Rosso[a]

a Dipartimento di Matematica and CNISM, Università di Pavia, via Ferrata 1, 27100 Pavia, Italy
b Marian Smoluchowski Institute of Physics, Department of Statistical Physics and Mark Kac Center for Complex Systems Research, Jagiellonian University, Reymonta 4, Kraków, Poland

Tetrahedral symmetry in nematic liquid crystals has been studied for several years, since the seminal paper by Fel[(1)]. Amongst statistical theories of nematic liquid crystals, a molecular mean-field model has proven to be quite effective in predicting phase sequences for thermotropic biaxial nematic molecules endowed with D_{2h} symmetry, as a function of the parameters entering their interaction potential[(2,3)]; this model has highlighted the role of a partially repulsive quadrupolar potential of mean torque in promoting condensed phases. It has been shown that the quadrupolar approximation to the excluded-volume interaction between hard spherocuboids can be written precisely as the superposition of two London interactions: one repulsive and one attractive[(4)]; furthermore, polar steric interactions have been shown to be capable of inducing orientationally ordered states possibly unexpected[(5)]. We compute analytically the excluded volume function for non-convex tetrahedral molecules, modelled as chains of tangent hard spheres. Since this function is overly complicated, we expand it over a suitable set of WSAFs (Wigner's Symmetry Adapted Functions).

References
(1) Fel, L.G. *Phys. Rev. E* **1995**, *52*, 702.
(2) Bisi, F.; Virga, E.G.; Gartland Jr, E.C.; De Matteis, G.; Sonnet, A.M.; Durand G.E. *Phys. Rev. E* **2006**, *73* , 051709.
(3) Bisi, F.; Luckhurst, G.R.; Virga, E.G. *Phys. Rev. E* **2008**, *78* , 021710.
(4) Rosso, R.; Virga, E.G. *Phys. Rev. E* **2006** *74* , 021712.
(5) Bisi, F.; Rosso, R.; Virga, E.G.; Durand, G.E. *Phys. Rev. E* **2008**, *78*, 011705.