

# A two-component mixture of Janus-like anisotropic sticky hard spheres

Miguel Ángel G. Maestre\* and Andrés Santos\*\*

*Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain*

Recently, the study of the physical properties of so-called Janus spheres (where half the surface is hard and the other half is sticky) has been the subject of much attention<sup>1</sup>. In the present work we study a closely related system composed by spheres of the same diameter but belonging to two different equimolar species. The surface of each particle is divided into fixed “North” and “South” hemispheres, one of them being stickier (North hemisphere for species 1, South hemisphere for species 2) than the other one. According to this, there are four possible forms of interaction between the particles and therefore four temperature-like stickiness parameters:  $\tau_{11}$ ,  $\tau_{12}$ ,  $\tau_{21}$  and  $\tau_{22}$ . In the case of a common value  $\tau_{11} = \tau_{12} = \tau_{21} = \tau_{22}$ , we recover the well-known Baxter sticky-hard-sphere (SHS) model, which is known to present a vapor-liquid critical point.

In our system we want to preserve the Janus-like feature of the model and thus we keep  $\tau_{12}$  (representing the interaction of a particle of species 1 being “below” a particle of species 2, so that the two respective stickier faces are in contact) different from  $\tau_{21}$  (representing the interaction of a particle of species 2 being “below” a particle of species 1, so that the two respective less sticky faces are in contact). Next, by symmetry, it is assumed that  $\tau_{11} = \tau_{22}$ . Two classes of models are considered:

- **Model A:**  $\tau_{12} = \tau$ ,  $\tau_{11} = \tau_{22} = \tau_{21} = \tau/\mu$ ,
- **Model B:**  $\tau_{12} = \tau_{11} = \tau_{22} = \tau$ ,  $\tau_{21} = \tau/\mu$ ,

where  $0 \leq \mu \leq 1$ . The introduction of the parameter  $\mu$  allows us to modify both the anisotropy of the system and the strength of the less sticky interaction, relative to the stickier interaction. Thus, both models A and B reduce to the conventional isotropic SHS model if  $\mu = 1$ . In the opposite limit  $\mu = 0$ , model A presents three HS and one SHS interactions, while model B presents one HS and three SHS interactions.

We have applied the rational-function approximation methodology<sup>2</sup> to generalize the analytical solution of the Percus–Yevick equation for a multi-component isotropic SHS system<sup>3</sup> to the anisotropic case. As a result, we get a closed quartic equation whose physical solution is identified as the one reducing to Baxter’s solution in the special case  $\mu = 1$ . For a given value of  $\mu$ , it turns out that the physical solution ceases to be real if (a)  $\tau$  is smaller than a certain critical value  $\tau_c$  and (b) the packing fraction  $\eta$  lies in a certain interval  $\eta_1(\tau) < \eta < \eta_2(\tau)$ . As  $\tau$  tends to  $\tau_c$  from below, both  $\eta_1(\tau)$  and  $\eta_2(\tau)$  tend

to a common critical value  $\eta_c$ . Figure 1 shows the critical values  $\tau_c$  and  $\eta_c$  versus the ratio  $\mu$  for models A and B. In both cases the critical values  $\tau_c$  and  $\eta_c$  monotonically decrease until vanishing in the limit  $\mu \rightarrow 0$ . This signals the absence of critical behavior as soon as one of the four possible interactions in the equimolar mixture becomes non-sticky.

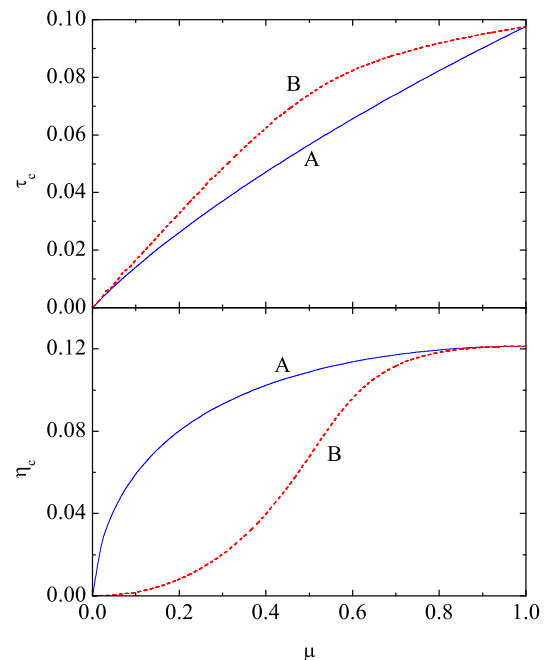


FIG. 1. Plot of  $\tau_c$  (top panel) and  $\eta_c$  (bottom panel) versus  $\mu$  for models A (solid blue lines) and B (red dashed lines).

\* maestre@unex.es

\*\* andres@unex.es

<http://www.unex.es/eweb/fisteor/andres>

<sup>1</sup> R. Fantoni, A. Giacometti F. Sciortino, and G. Pastore, *Soft Matter* **7**, 2419 (2011).

<sup>2</sup> M. López de Haro, S. B. Yuste, and A. Santos, in *Theory and Simulation of Hard-Sphere Fluids and Related Systems*, Lectures Notes in Physics, vol. 753, A. Mulero, ed. (Springer, Berlin, 2008), pp. 183–245.

<sup>3</sup> J. W. Perram and E. R. Smith, *Chem. Phys. Lett.* **35**, 138 (1975).