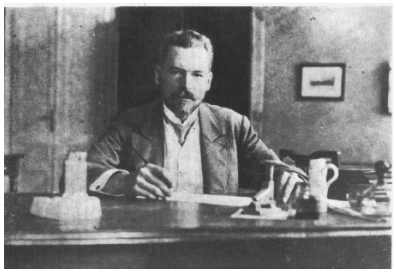

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How to use liquid state theory to predict jamming of hard spheres

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Slow compression of a hard-sphere fuid at constant temperature yields an entropy-driven first-order transition from the liquid to a crystalline phase [1, 2]. When the fuid is compressed quickly rather than slowly, however, crystallization can be avoided and the particles "jam" in a disordered configuration. The determination of the so-called *random close packing* (RCP) density, defined as the highest packing fraction for a disordered arrangement of hard spheres, remains an open problem [3].

In a recent paper [4], it was attempted to use liquid-state theories to analytically determine the RCP density of a monodisperse hard-sphere fluid. After combining a well-defined criterion for the onset of shear rigidity at jamming with a direct quantitative link between the contact value of the radial distribution function $g(r)$ and the kissing number z; existing equations of state for hard spheres were shown to be succesfull in predicting the RCP density either in $d = 2$ and $d = 3$ dimensions.

Here [5], we back up the analytical scheme introduced in [4]. We show that, when the notion of maximally random jammed (MRJ) state [3, 6] is generalized to that of MRJ-line, the Percus-Yevick and Carnahan-Starling equations of state capture the density dependence of z for a family of numerically generated jammed states of hard spheres. Consequently, it is reasonable to assume the most random branch of jammed states to undergo crowding in a way qualitatively similar to an equilibrium liquid. We prove that, for hard-sphere systems, liquid-state theories can be succesfully used to estimate RCP, when the latter is identified with the densest isostatic point, i. e. the densest among the MRJ states with $z = 6$.

Our finding is further enforced by the analysis of polydisperse systems. Either in the case of bidisperse and polydisperse hard spheres our prediction of RCP is in very good agreement with simulations, for a large values of size ratios and polydispersity. Finally, a perturbative expansion yields a closed-form expression for RCP that quantitatively captures a distribution-independent regime for small size polydispersities.

[1] W. W. Wood and J. D. Jacobson, The Journal of Chemical Physics **27**, 1207 (1957).
[2] B. J. Alder and T. E. Wainwright, The Journal of Chemical Physics **27**, 1208 (1957).
[3] S. Torquato and F. H. Stillinger, Reviews of Modern Physics **82**, 2633 (2010).
[4] A. Zaccone, Physical Review Letters **128**, 028002 (2022).
[5] C. Anzivino, M. Casiulis, T. Zhang, S. Martiniani, A. S. Moussa, and A. Zaccone, The Journal of Chemical Physics **158**, 044901 (2023).
[6] S. Torquato, T. M. Truskett, and P. G. Debenedetti, Physical Review Letters **84**, 2064 (2000).

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