Erratum: Explicit Analytical Solution for Random Close Packing in d=2 and d=3 [Phys. Rev. Lett. 128, 028002 (2022)]

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In this Erratum we wish to clarify a few statements contained in our Letter. First of all, the theoretical work contains an analytical solution to the random close packing (RCP) problem in both 2D and 3D. This solution is analytical and in explicit closed form, however, it cannot be regarded as exact (unlike, e.g., replica theory results which are exact in infinite dimensional systems [1]).

In particular, the method uses the Percus-Yevick (PY) solution for the contact value of the radial distribution function $g(\sigma^+)$. This is an approximation, because the PY solution for the full g(r), like other liquid-theory approaches, quoting from our Letter, "are unable to predict the divergence of pressure at RCP, and also cannot predict the formation of permanent nearest-neighbor contacts at RCP".

The PY solution is an approximation that remains formally valid all the way up to $\phi = 1$ (a physically inaccessible state), where the direct correlation function c(r) develops a pole. As recognized in [2], in this Letter we took advantage of this fictitious translationally invariant state, which contains no information about freezing, jamming, or packing, to construct an approximate solution.

Furthermore, the PY prediction for the g(r) presents other problems like negative parts for $\phi > 0.62$ [3], but this is immaterial for our derivation since it does not affect the contact value $g(\sigma^+)$. The latter remains positive and monotonically grows with ϕ , thus providing an effective, approximate way of statistically estimating the degree of crowding as the packing density increases [2].

It should be clarified that, in our derivation, one is certainly not attempting to describe the "real" g(r) of the metastable fluid, which is an enormously difficult task even for sophisticated numerical simulations. According again to [2], what is needed, to construct an approximate analytical solution, is just some underlying, fictitious uniform state, extending over the whole density domain, which has a g(r) that captures the increased crowding upon compression and densification. While it is even immaterial whether this state truly exists, possible inaccuracies in the approximation for $g(\sigma^+)$ are indeed effectively compensated by the choice of an ordered reference state to determine the unknown dimensionful constant g_0 [2]. The different values of g_0 and of ϕ_{RCP} that are obtained using different choices for the $g(\sigma^+)$ approximation and for the ordered reference state are summarized in Table I.

Finally, another statement in our Letter should be rectified: "The new method introduced above can be easily extended in future work to dimensions d > 3." It is in fact unclear how well our method holds as dimension is increased. Already at d = 8 a solution for RCP based on kissing contacts and marginal stability [4] like ours may not be adequate. For instance, it is known that in d = 8 there is a large jump between nearest neighbors even at the closest packing [5]. This is because in d = 8 one gets $4\binom{8}{2} + 2^7 = 112 + 128 = 240$ particles that pack $\sqrt{2}$ away from the origin and from each other (those happen to be the 240 root vectors of the eight-dimensional Euclidean E_8 Lie group) [5].

None of the above considerations affect the mathematical derivations and main physical conclusions of our Letter.

TABLE I. Values of normalization prefactor g_0 and random close packing density ϕ_{RCP} obtained using either the Percus-Yevick (PY) or Carnahan-Starling (CS) approximation schemes for $g(\sigma^+)$ and with different choices of ordered reference state for the effective boundary condition, i.e., body centered cubic (bcc) or face centered cubic (fcc).

	PY + fcc	PY + bcc	CS + fcc	CS + bcc	
$rac{10^2 g_0/\sigma}{\phi_{ m RCP}}$	3.318 94 0.658 963	3.740 68 0.643 320	1.874 16 0.677 376	2.429 46 0.650 594	

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