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Inverse melting and phase behaviour of core-softened attractive disks

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We use several computer simulation techniques to study the phase behaviour of a simple, two dimensional model that was originally devised to understand the anomalous properties of liquid water and their connection to a hypothesized liquid-liquid critical point. The interaction potential of this one-component system comprises a repulsive shoulder and an attractive square well. In our phase diagram of the model we find that the system exhibits inverse melting, for which the system crystallizes upon isobaric heating, over a small range of pressure [1]. We find that the range of pressures over which inverse melting occurs can be enlarged by increasing the extent of the repulsive shoulder [2]. Although our study is in 2D, we find that the transition is first order and to a liquid, rather than to a hexatic or quasicrystal phase. The increase in the range of inverse melting results in a change in the topology of the phase diagram, leading to further interesting behaviour.

[1] A. M. Almudallal, S. V. Buldyrev, and I. Saika-Voivod, J. Chem. Phys. 137, 034507 (2012).

[2] A. M. Almudallal, S. V. Buldyrev, and I. Saika-Voivod, arXiv:1401.0679 (2014).

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