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TWO-DIMENSIONAL CRYSTALLISATION ON SPHERICAL SURFACES

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ABSTRACT

We report results of a computational study on 2D crystallisation for a 25-particle Lennard-Jones system on a spherical surface, as a function of radius. The energy is minimised using simulated annealing and steepest descent methods. Different crystalline arrangements with clear energy minima are found at different radii. Qualitatively, most of the observed phenomena are representative also for systems with much larger numbers of particles.

1 Introduction

Spherical boundary conditions can be used as an alternative to periodic boundary conditions to approximate 2D bulk systems at sufficiently high temperature. However, crystallisation is affected in an essential way by any curvature of the 2D geometry. Specifically, phase transitions are expected to be influenced by curvature, because of the introduction of topological defects. These defects themselves tend to "crystallise", i.e. form regular patterns under spherical curvature. Crystalline arrangements on a spherical surface can also be of help to understand the arrangements in certain natural systems, for example bucky balls, sunflowers and viruses.

Using computer simulations we study 2D N -particle systems with two-body Lennard-Jones (LJ) interactions on a spherically curved surface, with parametric variation of the radius, such that the radius is fixed for each energy minimisation. Intuitively we can expect different arrangements to exist at different curvatures. Since our LJ potential has a minimum at unit distance, this distance is energetically favoured for neighbouring particles. If the surface of the sphere is larger than typically N surface units, the particles flock together leaving part of the sphere open (see figure 1a). For a particular radius the true global minimum is reached. This radius, the equilibrium radius R_{eq} , is energetically most preferred by the system. It will be searched for by the system, minimising the global energy, if the radius is a free parameter.

In section 2 we summarise our computational approach in the simulations and in section 3 we present results for the $N = 25$ system. In section 4 we give a preliminary conclusion derived from our data.

2 Computational Approach

To study crystallisation we use a simulated annealing (SA) algorithm to obtain minimum energy arrangements. SA is an optimisation technique closely related to the physics of the system. In physical annealing a material is heated to a high temperature and then allowed to cool slowly. In principle, this algorithm can "guarantee" finding the global

energy minimum, but the time required for convergence increases rapidly with increasing number of degrees of freedom and/or local minima. We have adapted SA to model the crystallisation on a spherical surface and made a sequential and a parallel implementation [1]; both were used in the present study. In our SA algorithm a compromise is sought between running time and cooling rate. In practical cases one can never be sure that SA reaches the global minimum for the given free parameter space. Therefore we perform a number of SA runs with different random start configurations. After annealing, the system is usually - but not always - close to the global minimum. From there we use an iterative steepest descent (SD) algorithm, see [2] [3], to search for the nearest true minimum. The SD method seeks a balance of forces on the particles within a given tolerance.

We also use SD alone to investigate the energy behaviour of a certain topological arrangement as a function of the radius of curvature. We start from an arrangement obtained by SA+SD and change the radius in small steps. After each step the SD method is used to obtain the energy minimum at the new radius.

Figure 1 : a) The cap arrangement at $R=1.52$.
 b) The particle energies of the cap and global minimum.

3 Results

In this paper we illustrate some general properties of the crystalline phase on a spherical surface, using by way of example a system of $N = 25$ LJ-particles. This N -value is sufficiently small to allow us to perform a great number of simulation runs and it is relatively far from values with a built-in tendency for an obvious global symmetry, like $N = 20$ or 32 . Figure 2 shows the minimum energies obtained by applying SA and SD to random initial configurations on spheres with randomly chosen (fixed) radii. In this figure we see the global minimum at $R_{eq} = 1.37$. For $R < R_{eq}$ the system is compressed implying that the particles are pushed close to each other, where the LJ-potential has a repulsive core. For $R > R_{eq}$ the system loses all external constraints except those arising from the curved geometry of its configuration space. Those arrangements cannot be closed around the sphere and they form a cap as shown in figure 1a. Particles at the edge of the cap do not have the optimal number of neighbours. Their energy is consequently higher than for closed configurations near the global minimum. Figure 1b displays the single particle energies for all 25 particles at two different radii, the one corresponding to Figure 1a and the other to the arrangement at R_{eq} . Due to the specific choice of $N = 25$, the equilibrium arrangement does not even have two particles at the same energy, which implies a total lack of symmetry. However, the cap arrangement of figure 1a has a clear 3 fold global symmetry.

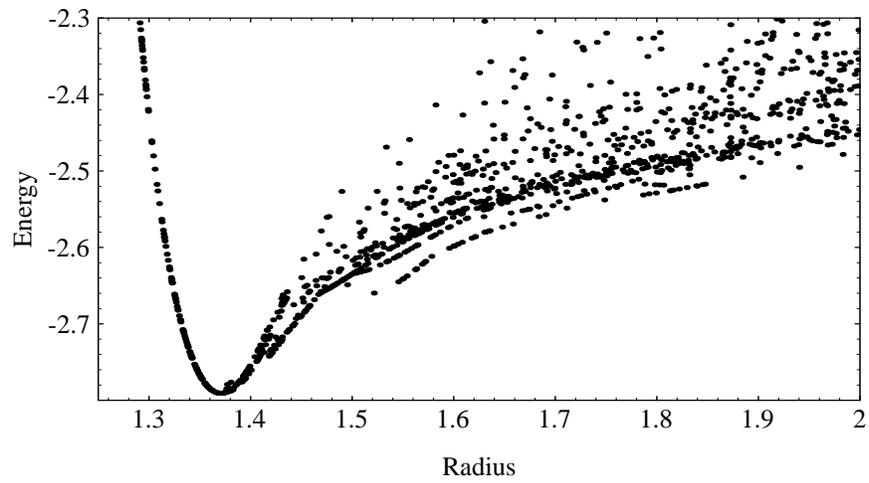


Figure 2 : The energies of the obtained arrangements.

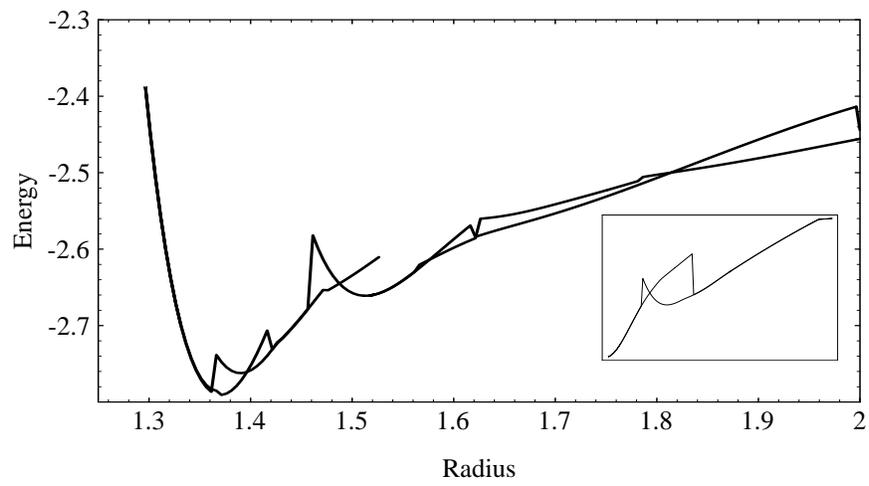


Figure 3 : Energy of an arrangement if the radius is changed.

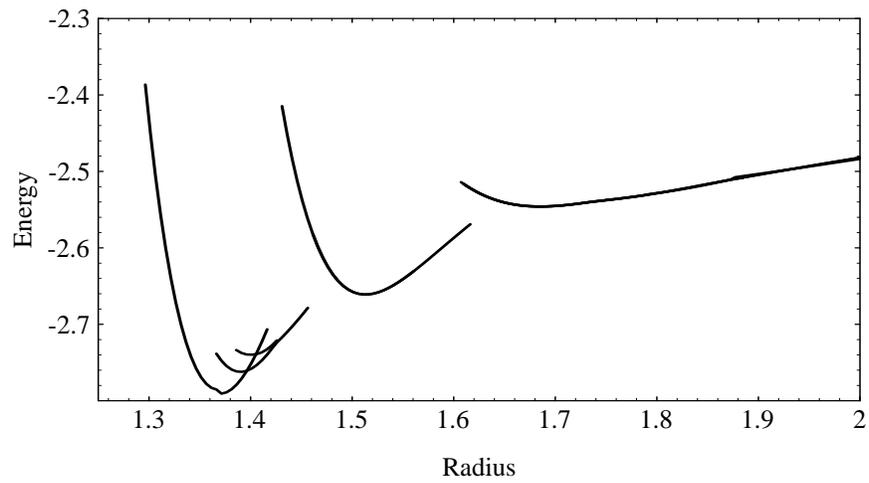


Figure 4 : A number of minima as a function of the radius.

We can see that the points, which correspond to energy minima obtained with the SA+SD procedure, form strings along curves. These lines correspond to (meta)stable topological arrangements. A curve below which no points fall, is clearly visible. This curve is the global minimum as a function of R . From the concentrations of the points we infer that the configuration with the lowest energy is not always the one with largest probability, for the particular set of random starts used.

The change of radius may also enforce a transformation to a new topological arrangement. If we take an arrangement from figure 2 and change the radius in small steps while the SD technique keeps the arrangement in a (meta)stable minimum, we observe that at certain points the arrangement is no longer stable. At those points the arrangement "breaks up" and the particles undergo a reordering in their positions until an arrangement is achieved that is stable at the new curvature. Figure 3 shows how the energy of an arrangement changes with R . Starting from the point at $R = 1.52$, we let R run up and down while applying SD until the system is back at the starting radius. An interesting curve is traced in this way with minima corresponding to different arrangements and sharp transitions between them. The inset shows a simple case. It is clear that there exists a re-arrangement barrier; the energy difference has to become large before the transition to a lower energy arrangement is realised. This causes the remarkable hysteresis effect. When the procedure described in the previous paragraph is applied to a number of arrangements we find that many of them exhibit a minimum in the energy-radius diagram. Prominent minima obtained in this way are shown in figure 4. When R is a free parameter, the system may be trapped in any of such minima.

4 Conclusion

As shown by our $N = 25$ LJ-study and in agreement with much larger spherical systems (N up to 1000), we find a number of different (meta)stable crystalline arrangements on a spherical surface, which correspond to certain energetically preferred values of R .

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