The high density phase of the $k$-NN hard core lattice gas model

Trisha Nath and R Rajesh

The Institute of Mathematical Sciences, C.I.T. Campus, Taramani, Chennai 600113, India
E-mail: trishan@imsc.res.in and rrajesh@imsc.res.in

Received 28 April 2016
Accepted for publication 21 June 2016
Published 11 July 2016

Online at stacks.iop.org/JSTAT/2016/073203
doi:10.1088/1742-5468/2016/07/073203

Abstract. The $k$-NN hard core lattice gas model on a square lattice, in which the first $k$ next nearest neighbor sites of a particle are excluded from being occupied by another particle, is the lattice version of the hard disc model in two dimensional continuum. It has been conjectured that the lattice model, like its continuum counterpart, will show multiple entropy-driven transitions with increasing density if the high density phase has columnar or striped order. Here, we determine the nature of the phase at full packing for $k$ up to 820302. We show that there are only eighteen values of $k$, all less than $k = 4134$, that show columnar order, while the others show solid-like sublattice order.

Keywords: classical phase transitions, phase diagrams
1. Introduction

Models of particles interacting through only hard core interactions are the simplest theoretical models to show phase transitions. All order-disorder transitions seen in such models are geometrical and entropy driven. A well-known example is the system of hard spheres \([1, 2]\). In three dimensions, it undergoes a discontinuous transition from a liquid phase to a solid phase with increasing packing fraction. In two dimensions, the freezing occurs in two steps: first from a liquid phase to a hexatic phase with quasi long range orientational order and second from the hexatic phase to a solid phase with orientational order and quasi long range positional order \([3–7]\).

The lattice version of the hard-sphere model, the \(k\)-NN model, has also been extensively studied since being introduced in the 1950s \([8–10]\) (also see \([11, 12]\) and references within for other applications). In this model, the first \(k\) next nearest neighbors of a particle are excluded from being occupied by another particle. On the triangular lattice, the 1-NN model reduces to the hard hexagon model, one of the few exactly solvable hard core lattice gas models \([13]\). In this paper, we focus on the continuum limit of the \(k\)-NN model on the square lattice. This corresponds to the limiting case of large \(k\), when it might be expected that the model converges to the hard sphere system in two dimensions.

We briefly summarize what is known about the different phases and phase transitions observed in the \(k\)-NN model on a square lattice. The 1-NN model, in which the nearest neighbor sites of a particle are excluded, undergoes a continuous transition belonging to the Ising universality class from a low density disordered phase to a high density solid-like sublattice phase with two-fold symmetry \([11, 14–32]\). The high density phase of the 2-NN model, also known as the \(2 \times 2\) hard square model, is columnar with translational order present only along either rows or columns but not along both \([15, 26, 33–43]\). The ordered phase has a four-fold symmetry and the transition is continuous and belongs to the Ashkin–Teller universality class \([11, 44, 45]\). The 3-NN model undergoes a discontinuous transition from the disordered to a sublattice phase with ten fold symmetry \([11, 15, 33, 35, 46–51]\). The 5-NN (\(3 \times 3\) hard square) model undergoes a first order transition into a columnar phase with 6 fold symmetry \([11]\).

In a recent paper, we showed numerically that the 4-NN model surprisingly undergoes two phase transitions as density is increased: first from a low density disordered
phase to an intermediate sublattice phase and second from the sublattice phase to a high density columnar phase [12]. The existence of two transitions was rationalized by deriving a high density expansion about the ordered columnar phase. Columnar phases have a sliding instability in which a defect created by removing a single particle from the fully packed configuration splits into fractional defects that slide independently of each other along some direction [15, 37, 52]. The high density expansion for the 4-NN model showed that the sliding instability is present in only certain preferred sublattices. As density is decreased from full packing, it is thus plausible that the columnar phase destabilizes into these preferred sublattices resulting in a sublattice phase rather than a disordered phase. This led us to conjecture that for a given $k$, if the model satisfies the two conditions (i) the high-density phase is columnar and (ii) the sliding instability is present in only a fraction of the sublattices, then the system will show multiple transitions. Implementing a Monte Carlo algorithm with cluster moves [53–55], we were able to numerically verify the conjecture for $k = 6, 7, 8, 9$, by showing the presence of a single first order transition, and for $k = 10, 11$ (for which the high density phase is columnar), by showing the presence of multiple phase transitions [12]. The results for $k \leq 11$ are summarized in table 1.

| $k$ | Ordered phases | Nature of transition |
|-----|----------------|---------------------|
| 1   | Sublattice     | Continuous (Ising)  |
| 2   | Columnar       | Continuous (Ashkin–Teller) |
| 3   | Sublattice     | Continuous         |
| 4   | Sublattice     | Continuous (Ising)  |
| 5   | Columnar       | Continuous         |
| 6   | Sublattice     | Continuous         |
| 7   | Sublattice     | Continuous         |
| 8   | Sublattice     | Continuous         |
| 9   | Sublattice     | Continuous         |
| 10  | Sublattice     | Continuous (Ising)  |
| 11  | Columnar       | Continuous         |

Note: More than one entry for a given value of $k$ indicates that multiple transitions occur with increasing density with the phases appearing in the order it is listed. Question marks denote that the result is not known.

The presence of multiple transitions in the $k$-NN model, which was hitherto unexpected, raises the intriguing possibility that in the continuum limit $k \rightarrow \infty$, the system may show multiple transitions as in the hard sphere problem in two dimensions. Monte Carlo simulations of systems with $k \geq 12$ is impractical as, at high densities, the large excluded volume per particle results in the system getting stuck in long lived meta stable states, making it a poor candidate for studying large $k$. Instead, in this paper, we find those values of $k$ for which the high density ordered phase is columnar by determining the configuration at full packing.

The rest of the paper is organized as follows. In section 2, we precisely define the model and the columnar and sublattice phases. In section 3, we explain the procedure for determining whether the high density phase has columnar order. Implementing this
The high density phase of the $k$-NN hard core lattice gas model

algorithm, we show that the number of system with columnar order is finite and that for large $k$, the high density phase has sublattice order. We conclude with discussions in section 4.

2. Model and definitions

Consider a square lattice with periodic boundary conditions. A site may be empty or occupied by utmost one particle. A particle in a $k$-NN model excludes the first $k$ next nearest neighbors from being occupied by another particle. Figure 1 shows the excluded sites for $k = 1, \ldots, 5$, where the label $n$ refers to the $n$th next nearest neighbor. We refer to this model as the $k$-NN model. As an example, only the nearest neighbors are excluded in the 1-NN model. With increasing $k$, the successive excluded regions correspond to lattice sites within circles of radius $R$, where $R^2$ are norms of the Gaussian integers.

Our conjecture states that for multiple phase transitions to be seen, the high-density phase should be columnar in nature and the sliding instability should be present in only a fraction of the sublattices. If the excluded volume is a perfect square oriented along the $x$- or $y$-axes, then the high density phase will be columnar, but the sliding instability will be present in all sublattices. However, the excluded volume is a hard square oriented along the axes only when $k = 2$ and $k = 5$. Thus, the conjecture reduces to determining for a given $k > 5$ whether the high density phase has columnar order. This may be determined by examining the fully-packed phase.

We now give an example of a columnar phase at full packing to identify a criterion to determine whether the fully packed phase has columnar order. Consider the 4-NN model whose high density phase has columnar order [12]. A typical configuration at

\[ \text{Figure 1. Consider a particle placed on the central black lattice site. The labels } n = 1 \text{ to } n = 5 \text{ denote the sites that are the } n\text{th next nearest neighbors of the particle. In the } k\text{-NN hard core lattice gas model all the sites with labels less than or equal to } k \text{ are excluded from being occupied by another particle. The excluded regions are also shown by concentric circles such that all sites within the circle of radius } R \text{ are excluded for a given } k. \]
The high density phase of the k-NN hard core lattice gas model

full packing is shown in figure 2. We divide the lattice into four sublattices depending on the diagonal that it belongs to. However, diagonals may be oriented in the $\pi/4$ direction or in the $3\pi/4$ direction and, thus, two such labelings are possible. In the configuration shown, all particles are in sublattice 2 when sites are labeled from 0 to 3 (see figure 2(a)), but in sublattices 4 and 6 when sites are labeled from 4 to 7 (see figure 2(b)). Clearly, there are 8 such phases possible. The key feature is that when boundary conditions are periodic, then the particles may slide freely along diagonals (red lines in figure 2), independent of other diagonals.

Thus, the degeneracy of the fully packed phase increases exponentially with system size.

In contrast, when the system has sublattice order, the number of fully packed configurations are finite. An example is the 1-NN model. In this case, the lattice may be divided into two sublattices such that neighbors of a site of one sublattice belong to the other sublattice (see figure 3). In the limit of full packing, all the particles are either in sublattice A or in sublattice B, and only two configurations are possible irrespective of system size.

Thus, we fix the the criterion for columnar order at full packing to be that the particles should be slidable along some direction (not necessarily $\pi/4$ or $3\pi/4$ as in 4-NN) independent of the positions of the other particles resulting in a highly degenerate fully packed state. In section 3, we describe the algorithm for checking slidability in the fully packed configuration.
Figure 3. The two sublattices for the 1-NN model are shown by $A$ and $B$. A fully packed configuration (shown by blue filled sites) consists of all particles being in sublattice $A$ (as shown in figure) or in sublattice $B$.

Figure 4. A schematic diagram to explain the procedure for constructing the unit cell at full packing. The unit cell is a parallelogram $ABCD$. The blue (filled) circles are particles. All lattice points inside the black and red circles are excluded by $A$ and $B$ respectively. If $C$ is placed on the lattice site denoted by white (open) circle, then the parallelogram has smaller area than the square $ABCD$. 
3. Results

To find the possible configurations for the $k$-NN model at full packing, we proceed as follows. The unit cell that repeats to give the fully packed configuration is a parallelogram. Let the particle at the top left corner of the parallelogram be denoted by $A$ (see figure 4). We choose the origin of the coordinate system to be at $A$. The excluded volume of $A$ is a circle (shown in black in figure 4) whose radius is dependent on $k$. Let the particle at the top right corner of the parallelogram be denoted by $B$ with coordinates $(x, y)$. We restrict the choice of $B$ to be in the first octant ($x \geq y$), as a choice in the second octant may be mapped onto the first octant by rotation. For every $y \geq 0$, $x$ is the minimum value such that $x^2 + y^2 > R^2$, where $R$ is the radius of the excluded volume. The excluded volume of $B$ is shown by a red circle in figure 4.

For a fixed $A$ and $B$, the orientation and length of the segment $CD$ is fixed as the unit cell is a parallelogram. The position of $C$ is determined by the constraint that the area of the parallelogram is the minimum and is determined as follows. A convenient initial choice of $C$ that does not violate the hard-core constraint is obtained by rotating the point $B$ counterclockwise about $A$ by $\pi/2$ such that the unit cell is a square (see figure 4). A choice of $C$ where $\angle BAC > \pi/2$ may be mapped onto a unit cell where $\angle BAC < \pi/2$ by translating the segment $CD$ by its length along its length. It is now straightforward to see that any choice of $C$ that results in a smaller area for the unit cell as compared to the initial square must lie within the initial square and outside the excluded volume of $A$ and $B$ (for example, the lattice point shown by an empty circle in figure 4). We fix $C$ by minimizing the area of the parallelogram over all such points.

The minimization of area is repeated over all possible choices of $B$ to determine the unit cell and the maximal packing density. If the segment $CD$ now passes through any lattice point that is outside the excluded volume of $A$ and $B$, then $C$ could be moved to that lattice point to give a parallelogram of same area. Likewise, if $AC$ passes through any lattice point that is outside the excluded volume of $B$ and $D$, then $A$ could be moved to that lattice point to give a parallelogram of same area. If such multiple choices are possible, then we identify the high-density phase to have columnar order.

Using the above procedure, we identify the fully packed configuration for $k$ up to 820 302 corresponding to $R^2 = 3999997$, where $R$ is the radius of the smallest circle.
The high density phase of the \( k \)-NN hard core lattice gas model

The number of distinct values of \( k \) increases linearly with \( R^2 \) (see figure 5(a)). Asymptotically we find \( k \approx 0.148 R^2 \), for \( R \gg 1 \). The values of \( k \) for which the high density phase has columnar order are listed in table 2. We find that up to the values of \( R^2 \) that we have checked, the largest \( k \) for which there is columnar order at full packing is \( k = 4183 \) or \( R^2 = 15482 \). Among these, the stability of columnar phase for density close to full packing has been numerically

| \( k \) | \( R^2 \) |
|---|---|
| 2 | 2 |
| 4 | 5 |
| 5 | 8 |
| 10 | 17 |
| 11 | 18 |
| 14 | 26 |
| 31 | 68 |
| 39 | 89 |
| 64 | 157 |
| 105 | 277 |
| 141 | 389 |
| 342 | 1040 |
| 427 | 1322 |
| 493 | 1557 |
| 906 | 3029 |
| 907 | 3033 |
| 4132 | 15 481 |
| 4133 | 15 482 |

Note: \( R \) is radius of the smallest circle that encloses the excluded lattice sites (see figure 1).

Figure 6. Wigner–Seitz cells for 6-NN and 13-NN models. Black dots are particles. The surrounding red circles are the exclusion regions of the central particle A. Blue lines are the perpendicular bisectors on the lines joining neighboring particles to A. Wigner–Seitz cell is a (a) square for 6-NN, (b) hexagon for 13-NN.

around a site that encloses all its excluded lattice sites. The number of distinct values of \( k \) increases linearly with \( R^2 \) (see figure 5(a)). Asymptotically we find \( k \approx 0.148 R^2 \), for \( R \gg 1 \). The values of \( k \) for which the high density phase has columnar order are listed in table 2. We find that up to the values of \( R^2 \) that we have checked, the largest \( k \) for which there is columnar order at full packing is \( k = 4183 \) or \( R^2 = 15482 \). Among these, the stability of columnar phase for density close to full packing has been numerically
established only for $k = 2, 4, 5, 10, 11$ [11, 12, 37]. Let $n_c(R)$ denote the number of systems whose exclusion is less than or equal to $R$ and has columnar order at full packing. $n_c$ increases irregularly with $R$ and saturates at $n_c = 18$ (see figure 5(b)).

For large $k$, the fully packed configuration has sublattice or crystalline order. For each of this $k$ we construct the Wigner–Seitz primitive cell obtained by constructing the convex envelope of the perpendicular bisectors of the lines joining a fixed particle to all other particles in the fully packed configuration. If the unit cell $ABCD$ is such that $\angle BAC$ equals $\pi/2$, then the Wigner–Seitz cell and the unit cell $ABCD$, are both squares. We find that the Wigner–Seitz cell is a square only for $k \leq 6$ and for $k = 11$. The Wigner–Seitz cell for 6-NN is shown in figure 6(a).

Figure 7. The dependence on exclusion radius $R$ of (a) angles $\alpha_i$, (b) ratios of lengths of different sides, and (c) ratio of area of the circumscribed circle to area of the hexagonal Wigner–Seitz cell.
For other values of $k$, we observe that $\angle BAC$ of the unit cell is always smaller than $\pi/2$. Also the length of the two sides, $AB$ and $AC$, are unequal. For these $k$, the Wigner–Seitz cell is an irregular hexagon where the opposite sides are parallel and of same length. Thus, pairs of opposite angles of the hexagon are equal to each other. As an example, the Wigner–Seitz cell for 13-NN is shown in figure 6(b).

We now characterize the shape of the Wigner–Seitz cell. Let the angles of the hexagon be denoted by $\alpha_1$, $\alpha_2$ and $\alpha_3$, such that $\alpha_1 \leq \alpha_2 \leq \alpha_3$. As $R \to \infty$, the three angles approach $2\pi/3$ linearly with decreasing $1/R$ (see figure 7(a)).

Likewise, let $l_1$, $l_2$, and $l_3$ denote the lengths of the hexagon such that $l_1 \leq l_2 \leq l_3$. The ratios $l_1/l_2$ and $l_3/l_2$ approach 1 linearly with decreasing $1/R$ (see figure 7(b)). We thus conclude that the Wigner–Seitz cell converges to a regular hexagon with increasing $k$.

We also check that in the limit of large $R$, the packing approaches that of discs in two dimensions. For discs, the largest packing density is achieved when the packing is hexagonal close packing with packing density $\eta = \pi/(2\sqrt{3})$. In the limit of large $R$, the ratio of the area of the largest circle circumscribed in the hexagonal Wigner–Seitz cell to the area of the hexagonal cell approaches $\eta$ (see figure 7(c)).

4. Conclusions

In this paper we obtained the nature of the phase at maximal density for the $k$-NN model hard core lattice gas models in which the first $k$ next nearest neighbor sites of a particle are excluded from being occupied by other particles by finding out numerically the configuration that maximizes the density at full packing. We find that for up to $k = 820\,302$, there are only 18 values of $k$ for which the high density phase has columnar order. The remaining ones have solid-like sublattice order. For these systems, we showed that the Wigner–Seitz primitive cell approaches a regular hexagon for large $k$, and the packing tends to a hexagonal packing.

The largest value of $k$ for which we found columnar order is $k = 4133$. Since this is 200 times smaller than the maximum value of $k$ that we have tested, it appears reasonable to conclude the number of systems with columnar order is finite.

If the conjecture that multiple transitions exist only if the high density phase is columnar [12] is true, then we conclude that for large $k$, the system shows one first order transition to a phase with sublattice order. In this case, the analogy to the hard disc problem in the two dimensional continuum, for which there are two transitions, breaks down. It would be interesting to test the conjecture more rigorously. One possibility is that even for systems with sublattice order, there could be two transitions. To show this, one needs to construct the high density expansion about the sublattice phase for large $k$ and check whether certain defects are preferred over others.

References

[1] Alder B J and Wainwright T E 1962 Phys. Rev. 127 359–61
[2] Alder B J and Wainwright T E 1957 J. Chem. Phys. 27 1208–9
[3] Kosterlitz J M and Thouless D J 1973 J. Phys. C: Solid State Phys. 6 1181
[4] Nelson D R and Halperin B 1979 Phys. Rev. B 19 2457
The high density phase of the $k$-NN hard core lattice gas model

[5] Young A P 1979 Phys. Rev. B 19 1855–66
[6] Bernard E P and Krauth W 2011 Phys. Rev. Lett. 107 155704
[7] Wierschem K and Manousakis E 2011 Phys. Rev. B 83 214108
[8] Domb C 1958 Il Nuovo Cimento 9 9–26
[9] Burley D M 1960 Proc. Phys. Soc. 75 262
[10] Burley D 1961 Proc. Phys. Soc. 77 451
[11] Fernandes H C M, Arenzon J J and Levin Y 2007 J. Chem. Phys. 126 114508
[12] Nath T and Rajesh R 2014 Phys. Rev. E 90 012120
[13] Baxter R J 1980 J. Phys. A: Math. Gen. 13 L61
[14] Gaunt D S and Fisher M E 1965 J. Chem. Phys. 43 2840–63
[15] Bellemans A and Nigam R K 1967 J. Chem. Phys. 46 2922–35
[16] Baxter R J, Enting I G and Tsang S K 1980 J. Stat. Phys. 22 465–89
[17] Baram A and Fixman M 1994 J. Chem. Phys. 101 3172–8
[18] Rummels L K 1965 Phys. Rev. Lett. 15 581–4
[19] Rummels L K and Combs L L 1966 J. Chem. Phys. 45 2482–92
[20] Ree F H and Chesnut D A 1966 J. Chem. Phys. 45 3983–4003
[21] Nisbet R and Farquhar I 1974 Physica 76 259–82
[22] Guo W and Blöte H W J 2002 Phys. Rev. E 66 046140
[23] Pearce F A and Seaton K A 1988 J. Stat. Phys. 53 1061–72
[24] Chan Y B 2012 J. Phys. A: Math. Theor. 45 085001
[25] Jensen I 2012 J. Phys. A: Math. Theor. 45 508901
[26] Binder K and Landau D P 1980 Phys. Rev. B 21 1941–62
[27] Meirovitch H 1983 J. Stat. Phys. 30 681–98
[28] Hu C K and Mak K S 1989 Phys. Rev. B 39 2948–51
[29] Liu D J and Evans J W 2000 Phys. Rev. B 62 2134–45
[30] Lafuente L and Cuesta J A 2003 Phys. Rev. E 68 066120
[31] Rácz Z 1980 Phys. Rev. B 21 4012–6
[32] Hu C K and Chen C N 1991 Phys. Rev. B 43 6184–5
[33] Bellemans A and Nigam R K 1966 Phys. Rev. Lett. 16 1038–9
[34] Ree F H and Chesnut D A 1967 Phys. Rev. Lett. 18 5–8
[35] Nisbet R M and Farquhar I E 1974 Physica 73 351–67
[36] Lafuente L and Cuesta J A 2003 J. Chem. Phys. 119 10832–43
[37] Ramola K and Dhar D 2012 Phys. Rev. E 86 031135
[38] Schmidt M, Lafuente L and Cuesta J A 2003 J. Phys.: Condens. Matter 15 4695
[39] Amar J, Kaski K and Gunton J D 1984 Phys. Rev. B 29 1462–4
[40] Slote P A 1983 J. Phys. C: Solid State Phys. 16 2935
[41] Kinzel W and Schick M 1981 Phys. Rev. B 24 324–8
[42] Ramola K, Damle K and Dhar D 2015 Phys. Rev. Lett. 114 190601
[43] Nath T, Dhar D and Rajesh R 2016 Europhys. Lett. 114 10003
[44] Feng X, Blöte H W J and Nienhuis B 2011 Phys. Rev. E 83 061153
[45] Zhitomirsky M E and Tsunetsugu H 2007 Phys. Rev. B 75 224416
[46] Bellemans A and Orban J 1966 Phys. Rev. Lett. 17 908
[47] Orban J and Van Belle D 1982 J. Phys. A: Math. Gen. 15 L501
[48] Nisbet R and Farquhar I 1974 Physica 76 283–94
[49] Heilmann O J and Praestgaard E 1974 J. Phys. A: Math. Nucl. Gen. 7 1913
[50] Eisenberg E and Baram A 2005 Europhys. Lett. 71 900
[51] Fiore C E and da Luz M G E 2013 J. Chem. Phys. 138 014105
[52] Nath T, Kundu J and Rajesh R 2015 J. Stat. Phys. 160 1173–97
[53] Kundu J, Rajesh R, Dhar D and Stilck J F 2012 AIP Conf. Proc. 1447 113–4
[54] Kundu J, Rajesh R, Dhar D and Stilck J F 2013 Phys. Rev. E 87 032103
[55] Kundu J and Rajesh R 2014 Phys. Rev. E 89 052124

doi:10.1088/1742-5468/2016/07/073203