The hard-core lattice gas

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We give an overview of the hard-core lattice gas, a statistical model of particles in a lattice which are forbidden to occupy adjacent sites. After an observation that this model obeys Ising universality, we consider two different approximations of the model: a mean-field theory, and a transfer matrix method where one of the dimensions is periodic.

I. INTRODUCTION

In this paper we will discuss the *hard-core lattice gas*, a simple model of a lattice gas with surprisingly complex behavior. In its simplest form, which is also the form that we will focus on, it concerns arrangements of particles on a square lattice, where each site can either be occupied or not. The defining feature of the model, which is also the reason for the name "hard-core", is that arrangements where two adjacent sites are both occupied are forbidden. Thus, one can view the particles as rigid, where moving two particles too close incurs an infinite energy penalty. All valid arrangements are weighted by $e^{\mu M}$, where M is the number of particles and μ is the chemical potential.

As one might expect from its simplicity, this model has many connections to other models. Mathematically speaking, a valid arrangement of particles is the same as an independent set of the grid graph encoding the adjacencies of the square lattice, so the partition function Z can be considered as a weighted enumeration of such sets. Also, it is possible to map the hard-core lattice gas onto the Ising model. Namely, if we let $\sigma_i = -1$ represents the absence of a particle at site i and $\sigma_i = 1$ represents presence, the hard-core lattice gas can be described via the Hamiltonian $-\beta\mathcal{H} = \sum_{\langle i,j\rangle} K(\sigma_i+1)(\sigma_j+1) + \sum_i \frac{\mu}{2}(\sigma_i+1)$ as $K \to -\infty$. This is equivalent to the Ising Hamitonian $-\beta\mathcal{H} = \sum_{\langle i,j\rangle} K\sigma_i\sigma_j + \sum_i h\sigma_i$ where $h = \mu/2 + 2K$.

It might not be initially clear why there might even be a phase transition, so we will first give a qualitative description. As expected, as μ increases the density ρ also increases, where we define ρ to the be fraction of sites that are occupied. In the limit where μ is very small, the repulsion of the particles is largely negligible, so the distribution of particles is disordered. On the other hand, if μ is very large, the particles arrange into a configuration that maximizes ρ, namely, a checkerboard sublattice which achieves $\rho = 1/2$. In particular, there must be some μ_c where long-range order appears. (Since the symmetry-breaking is discrete, there are no Goldstone modes to destroy long-range order.)

In this paper, we will first argue that this model must belong to the same universality class as the 2D Ising model. Since the 2D Ising model has been solved exactly on the square lattice, this result will provide crucial information regarding this system's critical exponents. We will then explore the relationship between μ and ρ using two different perspectives. First, we will use a mean-field theory to estimate the μ-ρ curve. Finally, we will approximate the square lattice with an $L \times \infty$ lattice with periodic boundary conditions. We then solve this exactly using transfer matrices.

One of the first considerations of this phase transition was made by Gaunt and Fisher [2], who used several series expansions to locate the phase transition and to estimate $\beta \approx 1/8$ (the meaning of β here will be discussed in Section II), strongly suggesting Ising universality. These estimates were subsequently refined, with Todo and Suzuki [8] later calculating that $\nu = 1.0001 \pm 0.0003$ and $\beta = 0.1249999 \pm 0.0000001$. The mean-field model we will present is adapted from work of Heringa, Blöte, and Luijten [3]. Our transfer matrix model was first carried out by Runnels and Combs [6], with some optimizations based on [8]. Other techniques to analyze the hard-core lattice gas include renormalization [4] and functional measure theory [5].

The hard-core lattice gas is also part of a family of models called the k-NN models, where the k shortest possible differences between two particles are forbidden. For example, the 1-NN model is just the hard-core gas, while the 3-NN gas forbids particles at distances of 1, $\sqrt{2}$, and 2 times the lattice spacing. This concept also extends naturally to non-square lattices. Unlike the 1-NN case, the mechanics of these more complex systems are far more unknown and complex. For instance, it is possible for the system to undergo multiple phase transitions, and in other cases it can exist in a "semi-ordered" state where columns are rigid but free to slide past each other. Finally, the universality class is not necessarily Ising; for some models the calculated critical exponents appear to match Potts models [7]. In general, these generalized lattice gases are much more unknown, as the techniques mentioned here either break down or require considerably more computational power to achieve comparable precision [1].

II. ISING UNIVERSALITY

As the phase transition involves interaction of the two checkerboard sublattices, to capture it we must use order parameters that involve these lattices. Namely, let $x(\mathbf{r}), y(\mathbf{r})$ be the occupancy fractions of each of the two sublattices, so that $\rho = \frac{x+y}{2}$. Also let $m = x - y$.

Due to the symmetry between x and y, any Landau-

Ginzburg-type Hamiltonian must be agnostic to the sign of m. Then we may write

$$-\beta\mathcal{H} = \int d^2\mathbf{r}\Big(a\rho + b\rho^2 + \frac{t}{2}m^2 + um^4 + c\rho m^2 + \frac{K}{2}(\nabla\rho)^2 + \frac{L}{2}(\nabla m)^2 + \cdots\Big).$$

Since the phase transition occurs when one sublattice becomes favored over the other, we conclude that a phase transition occurs when the coefficient of m^2 changes sign, though that no longer happens at $t = 0$ due to the $c\rho m^2$ term. Therefore, our model can be thought of as a 2D Ising model coupled to a scalar field ρ. While it is possible to continue working directly with this model, perhaps by using a saddle point approximation, the results are not incredibly interesting and we will omit it here.

However, the fact that this Landau-Ginzburg Hamiltonian behaves equivalently to the Ising model is very useful in examining the critical behavior of the model. Letting $f = -\frac{1}{N}\ln Z$, where N is the number of lattice sites, it is straightforward to show $\rho = -\frac{df}{d\mu}$. On the other hand, by the solution to the Ising model it is also true that "heat capacity" $-\frac{d^2f}{d\mu^2}$ undergoes a logarithmic singularity. Therefore, we should expect

$$\rho(\mu_c + \delta\mu) = \rho_c - c\,\delta\mu\log|\delta\mu| + O(\delta\mu).$$

for some $c > 0$. The hard-core lattice gas also inherits the exponent $\nu = 1$ from the Ising model. Other critical exponents describe the behavior of the order parameter m. For example, the exponent $\beta = 1/8$ implies that $|x - y|$ grows with order $(\mu - \mu_c)^{1/8}$ for μ slightly above μ_c.

III. MEAN-FIELD THEORY

A crude way to approximate ρ as a function of μ assumes that at densities x, y, particles are scattered randomly within each sublattice. In particular, consider one particular arrangement of particles in a sublattice at density x. At an arbitrary site in the other sublattice, the probability that none of its neighbors are occupied is $(1-x)^4$. At chemical potential μ, the probability that that site itself is occupied is thus $\frac{1}{1+e^{-\mu}}(1-x)^4$. Call $g(x) = \frac{1}{1+e^{-\mu}}(1-x)^4$. Then we have shown that $y = g(x)$. Similarly, $x = g(y)$.

When μ is low, the equation $x = g(g(x))$ has only one solution a, so we must have $(x, y) = (a, a)$ (see Fig. 1). On the other hand, past some critical μ_c, there are three solutions $a < b < c$, where $g(a) = c$, $g(b) = b$, and $g(c) = a$. In this case, we find that $|g'(b)| > 1$. Therefore, in some sense the solution $(x, y) = (b, b)$ is unstable, since small fluctuations to x cause y to fluctuate more, and vice versa. As a result, the solution that is more likely to represent reality is $(x, y) = (a, c)$ or $(x, y) = (c, a)$. This constitutes a phase transition at μ_c.

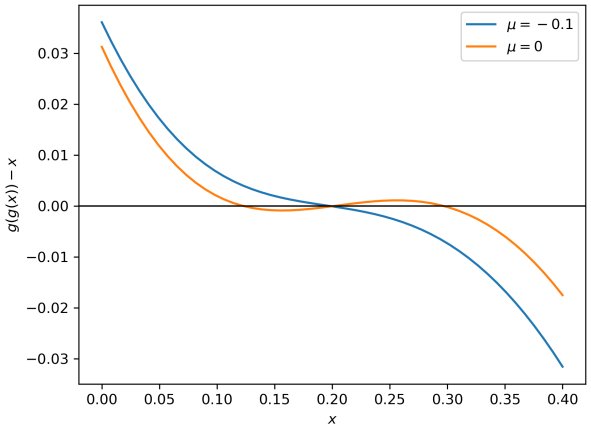

FIG. 1: Plot of $g(g(x)) - x$ for $\mu = -0.1, 0$.

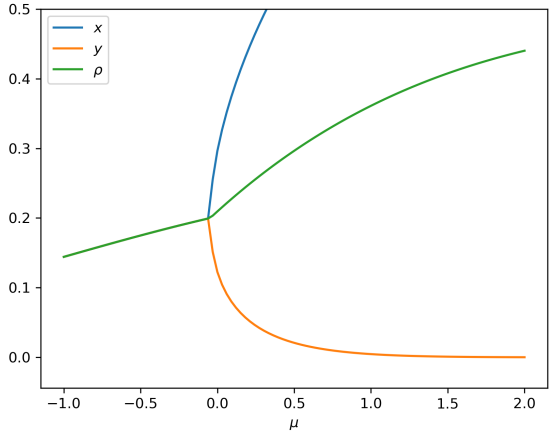

FIG. 2: ρ in the mean-field model.

The results of solving this system for various values of μ are found in Fig. 2. A phase transition occurs at $\rho_c = \frac{1}{5} = 0.2$ and $\mu_c = \ln\frac{125}{131} \approx -0.046$. As we will see later, the location of this critical point is rather inaccurate, though this mean-field model does become more accurate in higher dimensions [3]. As one might guess from the graph, $\frac{d\rho}{d\mu}$ has a jump discontinuity at μ_c, and since $C = -\frac{d^2f}{d\mu^2} = \frac{d\rho}{d\mu}$, we conclude $\alpha = 0$. Moreover, $\beta = 1/2$.

It is also possible to derive these exponents through calculation. At criticality, $g(x_c) = x_c$ and $g'(x_c) = -1$, so

$$\frac{d^2}{dx^2}g(g(x))\Big|_{x=x_c} = \frac{d}{dx}g'(g(x))g'(x)\Big|_{x=x_c} = g''(x_c)g'(x_c)^2 + g'(x_c)g''(x_c) = 0.$$

Thus, a good toy model for $g(g(x))$ is $(1-t)x + ax^3 + bx^4$, where we have translated so that $x_c = 0$ and $t = \mu - \mu_c$. If $t < 0$, then the only small solution to $x = (1-t)x +$

$ax^3 + bx^4$ is $x = 0$. However, if $t > 0$, then we must solve $t = ax^2 + bx^3$, which yields $x = \pm a^{-1/2} t^{1/2} + \frac{b}{2a^2} t + O(t^{3/2})$. The fact that $\beta = 1/2$ follows immediately from this expression. Also, we find that ρ is zero for $t < 0$ and $\frac{b}{a^2} t + O(t^{3/2})$ for $t > 0$, reproducing the jump discontinuity in $\frac{d\rho}{d\mu}$.

IV. TRANSFER MATRICES

Our final way of approaching the problem involves replacing the infinite square lattice with a $L \times \infty$ lattice that is only infinite in one dimension. We also impose periodic boundary conditions in the dimension of finite length.

In this circumstance, we can hope to compute Z directly with transfer matrices. Let $\mathcal{S}_L$ be the set of $\{0, 1\}$-vectors $S = (s_1, s_2, \ldots, s_L)$ so that s_i and s_{i+1} are not both 1 for all $1 \leq i \leq L$, where we take $s_{L+1} = s_1$. For $S \in \mathcal{S}_L$, let $|S|$ be the number of ones in S.

This setup now allows us to interpret a valid arrangement of particles on the lattice as a series of vectors $S_1, S_2, \ldots \in \mathcal{S}$, so that S_i and S_{i+1} do not share any ones at the same location. Each S_i contributes a weight of $e^{\mu |S|}$. Therefore, we conclude that

$$Z = \sum_{\{S_i\}} \prod_i T(S_i, S_{i+1}),$$

where the transfer matrix T is defined by

$$T(S, S') = \begin{cases} 0 & s_i = s'_i = 1 \text{ for some } i \\ e^{\mu(|S| + |S'|)/2} & \text{otherwise} \end{cases}.$$

As the lattice grows large, we conclude that $Z = \operatorname{tr} T^{N/L}$. Therefore, $f = -\frac{1}{N} \ln Z = -\frac{1}{L} \ln \lambda_0$, where λ_0 is the largest eigenvalue of T (which is positive by the Perron-Frobenius theorem). It is also true that $\xi^{-1} = \ln|\lambda_0/\lambda_1|$, where λ_1 is the second-largest eigenvalue.

In theory, taking arbitrarily large values of L would allow us to compute aspects of the hard-core lattice gas to arbitrary precision. In practice, though, $|\mathcal{S}_L| \sim (1.61803\ldots)^L$, so the time required to diagonalize the transfer matrix grows exponentially in L. Fortunately, there are still a few optimizations that make this task easier. For one, we have defined T to be symmetric, meaning that its eigenvectors are all orthogonal. There are several algorithms that take advantage of this fact to find the largest eigenvalues of T much faster than a full diagonalization. Also, it is possible to calculate Tv for some vector v using less memory than it would take to store T naïvely, which speeds up the process. In short, this is possible by, instead of moving directly from S to S', using several "hybrid" representations that combine parts of S and S' together (see [8] for more details).

We implemented this procedure with $L = 20$, which entailed diagonalizing 15127×15127 matrices. The results for ρ may be seen in Fig. 3. While it is a bit harder to detect than in the mean-field theory, a phase change can be seen at $\mu_c \approx 1.3$ and $\rho_c \approx 0.37$.

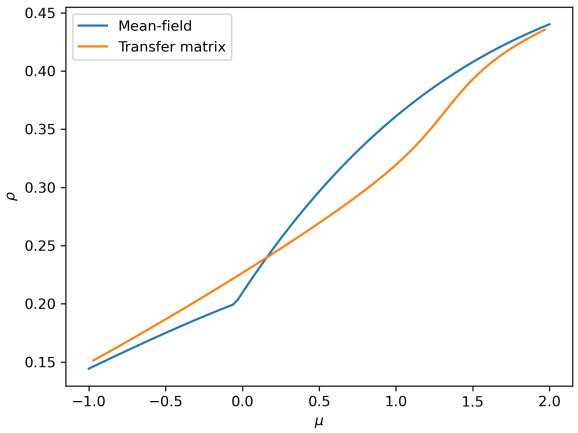

FIG. 3: Comparison of the mean-field and transfer matrix models.

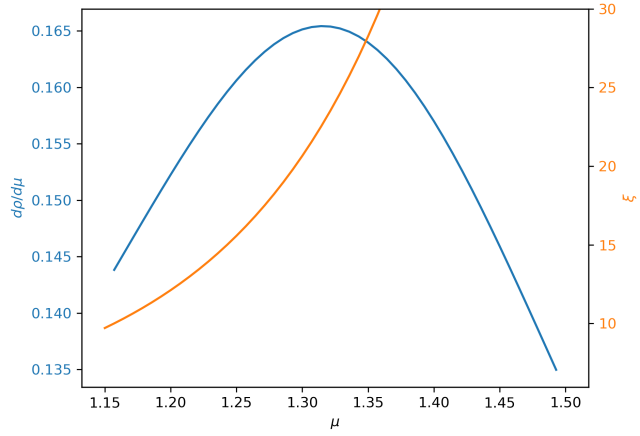

FIG. 4: Behavior around criticality for the $L = 20$ transfer matrix model.

Zooming in around the phase change, we find that it is characterized by a maximum in $d\rho/d\mu$ (see Fig. 4), which should approximate a logarithmic divergence. Moreover, we see a divergence of ξ. Since we set the length of one of the sides of the lattice to be L, a correlation length exceeding L signifies that the system is being affected by the periodic boundary conditions, meaning that the model is no longer reliable. Therefore, we should expect that $\xi \approx L$ near μ_c.

The value of μ that maximizes $d\rho/d\mu$ in this model is $\mu \approx 1.316$, which is close to the true value of $\mu_c \approx 1.3340$. A more sophisticated method to estimate μ_c can be used from the correlation length. Since the lattice gas has no characteristic scale at $\mu = \mu_c$, $\xi(\mu_c)$ can only depend on L. Thus, we should expect $\xi(\mu_c)/L$ to approach a fixed

value as $L \to \infty$ [8]. Setting $\xi_{L=18}(\mu)/18 = \xi_{L=20}(\mu)/20$, we find $\mu \approx 1.3343$, which is off by less than 10^{-3} from the true value.

V. CONCLUSION

In this paper, we have considered the hard-core lattice gas, a model, which like the Ising model, is very simple to describe and yet has a phase transition. While the Ising model describes the alignment of discrete magnetic spins via nearest-neighbor interactions, in the hard-core lattice gas particles "crystallize" from a disordered state into well-defined sublattices that permit greater packing densities. The fact that these two models have the same critical behavior is a reflection of the ubiquity of universality in the theory of phase transitions.

Although the critical behavior of the hard-core gas is crucial information, it does not tell us how to actually compute properties of the gas. In this paper, we implemented two different models to approximate this. First, we considered a mean-field theory, where a particle interacted with the aggregate of all sites of the opposite parity, instead of its immediate neighbors. In effect, we removed short-range order from the system. In this case, we observed a phase change that reproduced the critical behavior of the saddle point approximation to the Landau-Ginzburg Hamiltonian. This mean-field theory was reasonably accurate in determining ρ for large and small μ. However, the critical point predicted by the mean field model, $\mu_c = -0.046$, was very inaccurate.

Better results were achieved by making one of the dimensions of the lattice periodic of length L, allowing transfer matrices to be applied. Here, we saw evidence of a phase change near the theoretical value, with a noticeable spike in the heat capacity and a divergence of the correlation length. By comparing correlation lengths for different values of L, it is possible to improve estimates of μ_c to be within one part in a thousand of the theoretical value.

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