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Ground states of quasilattice-gas models

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Abstract

We introduce quasilattice-gas models in which every vertex of certain two-dimensional grids can be occupied by one of two different types of particles interacting through Lennard–Jones potentials. Such grids are quasiperiodic analogs of regular lattices present in periodic systems. To find ground-state configurations of our models, we performed Monte Carlo simulations and obtained structures with local five-fold symmetries and five-fold diffraction patterns. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Since the discovery of quasicrystals by Shechtman, Blech, Gratias, and Cahn in 1984 [1], one of the fundamental problems of condensed matter physics is to understand their occurrence in microscopic models of interacting particles. Equilibrium behavior of systems of many interacting particles results from the competition between energy and entropy, i.e. the minimization of the free energy. Therefore, the main goal is to show that equilibrium phases of certain atomic interactions possess some sort of quasicrystalline order. The first step is to exhibit some pair interactions which force quasicrystalline order in ground-state configurations (where at the zero temperature one has to minimize the energy of a given system). In [2–4], there were proposed certain interactions and then it was shown that the preferred quasiperiodic structures had lower energy density than some standard periodic lattices like fcc or bcc. One may also simulate the dynamical process of growing quasiperiodic structures using molecular dynamics [5–7] or Monte Carlo algorithms [8–10]. Here we follow the second approach.

A crucial observation for our numerical simulations is that vertices of tiles in almost all of two-dimensional geometrical models of quasicrystals, Bragg peaks of their diffraction patterns (beyond certain intensity) as well as the peaks of diffractions of real quasicrystalline materials and the actual positions of atoms in the micrograph pictures of such structures occupy sites of certain two-dimensional quasilattices. These quasilattices can strongly differ one from another but in almost all cases they can be embedded (after appropriate scalings) into a general 'canonical' structure called β-grid [11]. This latter quasilattice is based on β-integers, where, β is a Pisot–Vijayaraghavan unit (PVu) corresponding to certain n-fold symmetry.

To describe β-grids we first define β-integers. The regular integers $\mathbb{Z}$ are those with finite dyadic expansion:

$$\mathbb{Z} = \left\{ x \in \boldsymbol{R} | \exists_m \in N, \quad x = \pm \sum_{n=0}^{m} a_n 2^n, a_n \in \{0,1\} \right\}$$

In the complete analogy with the above expression, we define, for $\beta > 1$, $\beta \notin \mathbb{Z}$ the set of β-integers:

$$\mathbb{Z}_\beta = \left\{ \boldsymbol{R} \ni x = \pm \sum_{n=0}^{m} a_n \beta^n, \quad a_n \in \{0, 1, \ldots, [\beta]\}, \right. \\ \left. a_m, a_{m-1} \ldots a_0 \in W_\beta \right\}$$

Here $[\beta]$ is the integral part of β and W_β denotes the set of allowed words in the numeration system associated to β (see [12] for related definitions). Among many algebraic properties of β-integers, which were investigated in [12] for any quadratic PVu and in [13] for the simplest cubic PVu, their similarity under scaling $\mathbb{Z}_\beta \subset \mathbb{Z}_\beta / \beta$ is important in our quasilattice-gas scheme.

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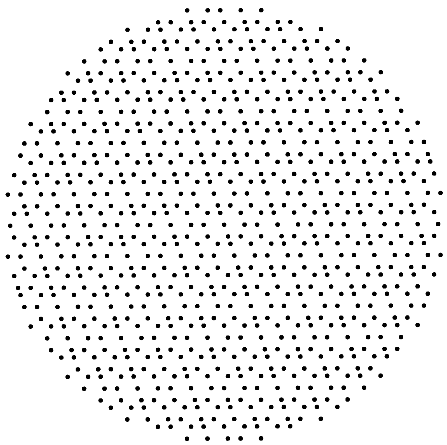

Fig. 1. Circular portion of the grid Γ_τ.

To accommodate structures with the five-fold symmetry, we set here $\beta=(1+\sqrt{5})/2\equiv\tau$ and we define the following two-dimensional grid:

$$\Gamma_\tau = \mathbb{Z}_\tau \otimes \mathbb{Z}_\tau e^{i\pi/5} \tag{1}$$

whose finite piece is shown in Fig. 1 and diffraction spectrum in Fig. 2. We will use Γ_τ as a background for interacting particles in the same way as the square lattice $\mathbb{Z}^2$ is used in ordinary lattice-gas models. Let us mention here that quasiperiodic ground-state configurations of particles occupying vertices of the regular square lattice were investigated in [14–16].

2. Quasilattice-gas models

In quasilattice-gas models, every site of Γ_τ can be occupied by one of two types of particles (a large disk-particle or a small disk-particle) *or be empty*. All infinite-quasilattice configurations are therefore elements of $\Omega=\{e, l, s\}^{\Gamma\tau}$, where e denotes an empty site, l the large particle, and s the small one. If $X\in\Omega$ and $\Lambda\subset\Gamma_\tau$, then we denote by X_Λ a restriction of X to Λ.

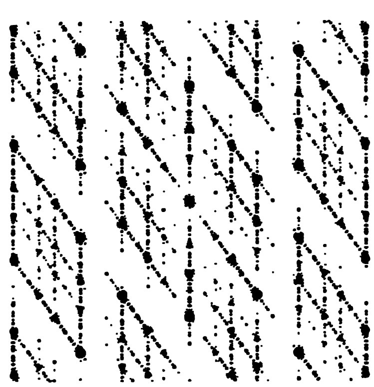

Fig. 2. Diffraction pattern of the grid of Fig. 1.

Particles interact through two-body symmetric *Lennard–Jones potentials*:

$$f_{\alpha,\beta}(r) = \epsilon_{\alpha,\beta}\left(\left(\frac{\sigma_{\alpha,\beta}}{r}\right)^{12} - 2\left(\frac{\sigma_{\alpha,\beta}}{r}\right)^{6}\right)$$

where $\alpha,\beta\in\{l, s\}$ and we set

$$\sigma_{l,l} = \sqrt{3-\tau}, \quad \sigma_{s,s} = \frac{1}{\tau}, \quad \sigma_{l,s} = 1$$

$$\frac{\epsilon_{l,l}}{\epsilon_{l,s}} = \frac{\epsilon_{s,s}}{\epsilon_{l,s}} = \frac{1}{2}$$

Such interactions were considered for instance in [9,10]. In [17,18], there were constructed binary-tilings models (tilings by two rhombi decorated with large and small particles) with nearest-neighbor interactions with strengths $-\epsilon_{\alpha,\beta}$ and diameters of particles $\sigma_{l,l}$ and $\sigma_{s,s}$ correspondingly. In all these papers, the relative densities of two types of particles were fixed.In terms of the above defined pair potentials, the Hamiltonian of our system in a bounded region $\Lambda\subset\Gamma_\tau$ is a sum over all pairs of sites contained in Λ

$$H_\Lambda(X) = \frac{1}{2}\sum_{(i,j)\in\Lambda} f_{X(i),X(j)}(|i-j|)$$

where $f_{X(i),X(j)}=0$ if $X(i)=e$ or $X(j)=e$.

Let us note here that the general theory of equilibrium states on quasicrystalline lattices was developed in [19]. In [20], the Pirogov–Sinai theory [21] was generalized to such systems.

Now our main task is to find *ground-state configurations* of our model. However, finding ground-state configurations even of simple Ising models is an extremely difficult task. Therefore, we resort here to Monte Carlo simulations.

3. Monte Carlo simulations

We restrict ourselves to a finite circular portion of the β-grid (2200 quasilattice sites) and we use a cut-off of the Lennard–Jones potential at a distance $r_c=5$. As an initial configuration we chose the one in which all sites of the grid are occupied by large particles. Let us observe that we work in the *grand-canonical ensemble*; we are not fixing densities of particles and we set chemical potentials to be zero for both types of particles. With that respect our models are different from other Monte Carlo simulations of quasicrystals [8–10].

We chose randomly a quasilattice site and assign to it a large particle, a small particle or leave it empty with probabilities corresponding to standard Boltzmann factors. This constitutes one step of our Monte Carlo algorithm (MC). The stationary state of such a stochastic dynamics is known to be an equilibrium state for given interactions and temperature. As temperature goes to zero, it is a small perturbation of ground states. Fig. 3 shows the resulting structure after one and half million steps. We see local structures with a

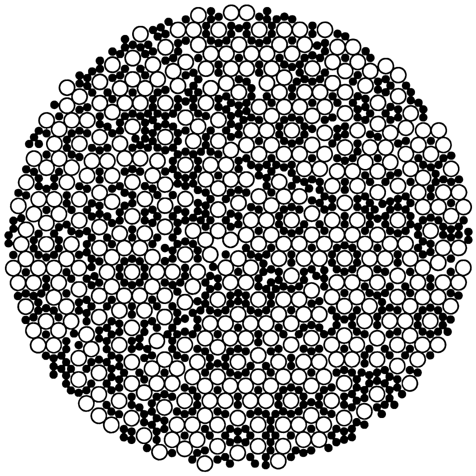

Fig. 3. Low temperature (T=0.5($\epsilon_{l,s}/k_B$) configuration after 1.6 Number of the big and small circles is N_l=392 and N_s=886.

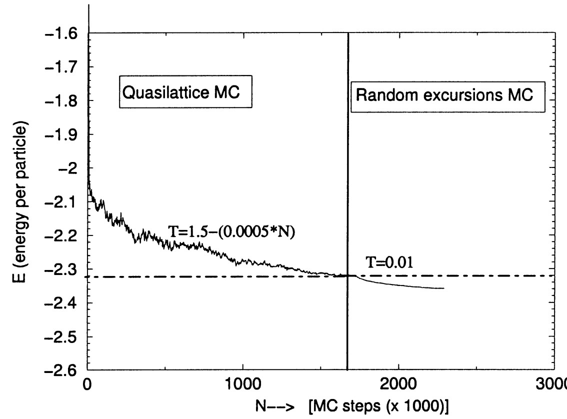

Fig. 5. Energy per particle measured in units of $\epsilon_{1,s}$ as a function of MC steps N (two different MC simulations). Cooling down is carried out by similar relaxation processes at several successive temperatures T (1.5 (0.0005×N)) $\varepsilon_{l,s}/k_B$.

five-fold symmetry consisting of two types of rhombi. The density of small particles is equal to p_s=0.4 and the density of large particles is equal to p_l=0.18; the ratio being approximately equal to $N_s/N_l = 2.26 \approx \tau + 1/\tau$. Let us notice that the above ratio (obtained by the minimization of the energy in the grand-canonical ensemble) is different from the one fixed in [8–10] to be approximately 1 in the canonical ensemble. We also calculated the diffraction spectrum of this structure. It is shown in Fig. 4.

Now to check the stability of our stationary structure we make our quasilattice structure thinner. We rescale distances between particles. Namely, we replace $\mathbb{Z}_\tau$ by $\mathbb{Z}_\tau/\tau$ (respectively, $\mathbb{Z}_\tau/\tau^2$) in (1), so density of occupied sites in the grid decrease by τ^2 (respectively, τ^4). We have not observed any qualitative changes both in the structure and its diffraction pattern as well as in the number of large and small particles. To approximate the continuum even further we should do further scalings. However, it would require an enormous amount of the computer time. Therefore, instead of this we perform *random-excursions* Monte Carlo simulations. More precisely, we take the result of quasilattice MC simulation as an initial configuration and we allow particles to deviate from the quasilattice. For each particle one defines a square of an excursion of size $b < \sigma_{\alpha,\beta}$ from the initial position. We randomly chose a particle and then two independent random numbers (from the uniform distribution) smaller than b which define the rectangular coordinates of the excursion. A new position of the particle is again accepted according to Boltzmann probabilities. In Fig. 5 we plot the graph of the total energy of the system as a function of number of steps, first in the quasilattice MC and secondly in the random-excursions MC simulations. We see a small (∼2%) decrease of the energy after the completion of the second MC process with respect to the first one. This was expected because the initial structure (the final structure of the quasilattice MC simulation) was not optimal. However, the smallness of the decrease together with the diffraction pattern confirms the stability of obtained quasicrystalline structure.

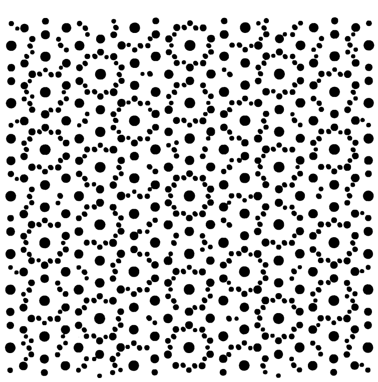

Fig. 4. Diffraction pattern of Fig. 3.

4. Conclusions

We introduced here quasilattice-gas models with two types of particles interacting through Lennard–Jones potentials. We performed Monte Carlo simulations and obtained quasiperiodic ground-state configurations with a local five-fold symmetry and five-fold symmetric diffraction patterns. The novelty of our approach is that we use quasilattices as filters to obtain stable configurations. We work in the grand-canonical ensemble; we do not fix densities of particles as it is done in other Monte Carlo simulations. We applied the same method to the model with one type of particles only and we obtained structures with crystalline order of the triangular lattice as is expected for ground states of the two-dimensional Lennard–Jones potentials. It would be important to investigate three-dimensional versions of our models. The work in this direction is in progress.

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