Random walks with sign reversals and the intrinsic angular momentum behaviour on lattices

C. Tresser, C. Brot, J. Coste

To cite this version:

HAL Id: jpa-00209027
https://hal.archives-ouvertes.fr/jpa-00209027
Submitted on 1 Jan 1981

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
Random walks with sign reversals and the intrinsic angular momentum behaviour on lattices

C. Tresser, C. Brot and J. Coste
Laboratoire de Physique de la Matière Condensée (*), Parc Valrose, Université de Nice, 06034 Nice Cedex, France

(Reçu le 7 juillet 1980, accepté le 20 novembre 1980)

Résumé. — On considère sur des réseaux des rotateurs classiques monoaxiaux n'échangeant du moment angulaire que dans un certain secteur d'orientation relative (secteur de collision), à cause de la portée supposée finie du potentiel anisotope d'interaction ; celui-ci peut d'ailleurs être supposé du type cœur dur (collisions instantanées). Les axes des rotateurs étant supposés parallèles mais non colinéaires, il est naturel de supposer que durant chaque collision, l'échange de moment angulaire est du type engrenage, c'est-à-dire se fait avec changement de signe.
Dans une première approximation, on néglige toute corrélation entre les collisions successives, ce qui revient à considérer une marche au hasard sur un réseau dans laquelle une variable attachée au marcheur change de signe à chaque transfert. On est alors amené à distinguer deux types de réseaux selon qu'un retour au site initial peut se faire par un nombre de déplacements élémentaires impair ou non.
Pour des réseaux bidimensionnels, on donne analytiquement la solution asymptotique du problème de la fonction d'autocorrélation du moment angulaire ainsi que son comportement aux temps plus courts obtenu numériquement. Pour des réseaux impairs, ce comportement asymptotique est, dans certaines conditions, exponentiel alors qu'il est algébrique pour les réseaux pairs.
Enfin, revenant au problème initial où les collisions successives sont interdépendantes, on donne quelques résultats de simulations numériques pour des réseaux bidimensionnels de molécules diatomiques à cœur mou (diatomiques de Lennard-Jones).

Abstract. — Classical uniaxial rotators on lattices are considered. The assumption is made that the rotators exchange angular momentum only in a certain sector of relative orientations (collision sector) because of the finite range of the anisotropic interaction potential ; the latter may in particular be a hard core potential (instantaneous collisions). Since the axes of the rotators are supposed to be parallel but not collinear, during each collision the exchange of angular momentum occurs with sign reversal, i.e. is of the cog-wheel type.
In a first approximation all correlations between successive collisions are neglected. This amounts to considering a random walk on a lattice in which the walker carries with him a variable whose sign is changed at each step. Then, one is led to distinguish two types of lattices, depending upon the possibility for returning to the initial site after an odd number of steps.
For two-dimensional lattices, the asymptotic solution of the autocorrelation function of the angular momentum is analytically given, and its behaviour at shorter times is obtained by a numerical method.
For the odd lattices, the asymptotic behaviour is generally exponential, whereas there exist algebraic long tails for the even lattices.
Finally, coming back to the problem where the successive collisions are not independent, some simulation results for two-dimensional lattices of soft core diatomics are described.

1. Introduction. — The kinetic theory of particles exchanging classical spins, i.e. intrinsic angular momentum during collisions, is not a trivial problem. This is due to the fact that total spin angular momentum is not conserved in a collision.
There can be different examples of this non-conservation. In fluids, part of the angular momentum transfer is exchanged with the vorticity. In models of rotatory crystalline phases, the centres of mass of the molecules are supposed to remain fixed. This amounts to assuming the existence of pivots, the reaction with which creates or annihilates a part of the angular momenta during the collisions.
As a consequence of the first example, in fluids, the hydrodynamics of local angular momentum has no obvious foundation. However, there exists in the literature a few theoretical [1] and experimental...
hints [2, 3, 4] about the behaviour of the Intrinsic Angular Momentum in fluids, expressed in the form of its time Autocorrelation Function (AMACF).

In particular, in a previous work performed by two of us [3, 4] (C.B. and C.T.) in collaboration with B. Quentrec, using numerical Molecular Dynamics simulation, a surprising $t^{-3} - b$ preasymptotic behaviour of the AMACF was observed in a 2-d diatomic fluid. (We recall that a modelled version of generalized hydrodynamics would predict a $t^{-2}$ decay in a 2-d system [1].) It was conjectured there that a cog-wheel mechanism, i.e. an intrinsic AM transfer with sign reversal (a typically non hydrodynamic one) was responsible for this behaviour. It seemed natural then to isolate this phenomenon by considering a dynamical system without vorticity. This can be done by considering models of rotationally free crystals (often called plastic crystals) as referred to above. A paper [5] was devoted to the numerical study of a one-dimensional plastic crystal consisting of a chain of rotators with fixed centres, two neighbouring particles exchanging their angular momenta with sign reversal

$$((\omega_1, \omega_2) \rightarrow (-\omega_2, -\omega_1))$$

in a collision. We observed in that work a dynamic of a diffusive character, with a AMACF decaying as $t^{-1/2}$; this is precisely the same law as that of a one-dimensional Brownian diffusion. We consider in this paper a 2-d version of this model, i.e. the dynamics of rotators fixed on the sites of a given lattice. Our results on the 1-d lattice suggest consideration of the associated problem of a random walk over the lattice, the connection with the initial dynamical problem being based on the fundamental assumption of independent successive collision events.

This random walk has a special and interesting feature: a dynamical quantity, namely the angular momentum, is carried along by the walker and changes sign at each interaction. This type of behaviour, which is studied in this paper, might be of more general interest than that of angular momentum transfers.

It appears that the properties of this random walk depend crucially on the parity of the lattice: a lattice being labelled odd or even according to whether there does (or does not) exist paths with odd number of steps leading the walker back to its initial site (this will be detailed in the next section). This concept is obviously related to those of lattices with or without frustration.

An important result of the analytic study of the random walks is that, asymptotically, AMACFs have an exponential decay in the case of odd lattices, as will be shown. This property also holds in a 3-d version of the model.

Such a property may be relevant in order to find a sound foundation of the hydrodynamics of angular momenta. We also observe, numerically, preasymptotic behaviour compatible with the $at^{-3} - b$ law [3, 4] in the 2-d lattice model.

2. A classification of lattices. — We assume throughout, as above [5]

$$((\omega_1, \omega_2) \rightarrow (-\omega_2, -\omega_1))$$

which means that if site $i$ has the AM $\omega$, before the collision, this value appears at site $j$ with its sign changed after the collision. Thus the AM $\omega$ walks randomly on the lattice, with a reversal of its sign at each step. For simplicity, and by realistic arguments, the sites $i$ and $j$ will often be supposed to be nearest neighbours on the lattice (not necessarily in a restricted geometrical sense, see below).

In section 4, we shall make a comparison between the theoretical results obtained in this idealized case and simulation results using Lennard-Jones diatomics where the collisions are ill-defined but nevertheless partially reverse the transferred angular momenta. Let us then consider the problem of the autocorrelation function of angular momentum for a 2-d lattice of molecules rotating in their common plane. We suppose an initial zero mean of the initial distribution of angular velocities. The numerical investigations we have done with such models suggest that, although the total AM is not a conserved quantity of the dynamical system, one finds that the long time average of angular momentum is zero. It remains then two effects which contribute to correlate angular momenta in time.

1) The persistence of the initial angular momentum on a site. This gives an exponential contribution to the AMACF.

2) The return of an angular velocity, possibly with a reversed sign, to its initial site. It is, in fact, remarkable that by equation (1) the norms of individual angular momenta are conserved and may thus be considered as quasiparticles.

It is clear then that the behaviour of the autocorrelation of angular momentum will depend strongly on whether or not a given velocity returns to its initial site after an odd number of collisions. This leads us to classify the lattices as odd or even, according to whether or not this possibility exists. A trivial remark is that even in odd lattices, returns can occur after an even number of collisions.

Let us now think of (1) in a more formal sense as representing any adequate abstract interaction. Then the problem can be generalized to any dimension, where we classify a lattice according to whether or not it allows, returns to the initial site after an odd number of interactions.

Let us emphasize that the word lattice here does not refer to a purely geometric structure but rather to the combination formed by a geometrical classical lattice (as e.g. in crystallography) and the list of sites that can interact directly with a given one. To clarify this point, let us consider the case of a geometric
square lattice and show how it gives different lattices in our sense. Around the origin \((0,0)\), let us denote by \((n_1, n_2)\) the site corresponding to \(n_1\) horizontal and \(n_2\) vertical unit displacements. We can denote a lattice (in our sense) by the list of sites interacting directly with \((0,0)\). Then \(\{(1,0),(0,1),(-1,0),(0,-1)\}\) gives the square lattice, an example of an even lattice. 

\[\{(1,0),(1,1),(0,1),(-1,1),(-1,0),(-1,-1),(0,1),(1,1)\}\] and \(\{(1,0),(0,1),(-1,0),(-1,-1),(0,1),(1,1)\}\) give examples of odd lattices, the second one being topologically equivalent to the triangular lattice with interactions between first neighbours.

We have represented, in figure 1, a table of some elementary examples of odd and even lattices, in one and two dimensions.

<table>
<thead>
<tr>
<th>EVEN</th>
<th>ODD</th>
</tr>
</thead>
<tbody>
<tr>
<td>One dimension</td>
<td></td>
</tr>
<tr>
<td>Two dimensions</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 1. — Some examples of odd and even lattices as defined in the main text. The arrows represent possible interactions for a given particle.

3. Random walks with sign reversal : the model. — We shall here construct probabilistic models of walks on lattices where it will be possible to determine analytically the long time behaviour of the AMACF, which will be denoted by \(F_{\omega}(t)\).

Before proceeding to this construction, let us describe a dynamical system for which the introduction of a probability distribution will provide the only idealization of our models. As has been seen at the end of the preceding section, some exotic lattices are topologically equivalent, for the dynamical problem at hand, to a square lattice. We shall hence restrict ourselves essentially to the \(d\)-dimensional hypercubic lattice \(\mathbb{Z}^d\) where \(d\) is the dimension of the space and \(\mathbb{Z} = \{\ldots, -2, -1, 0, 1, 2, \ldots\}\) is the set of all integers. This will provide us enough examples to illustrate the phenomena we wish to illustrate. We recall that in fact a lattice \(\mathcal{L}\) is the combination formed by some \(\mathbb{Z}^d\) and the list \(L\) of the interacting sites. On the other hand, the shape of the molecules is supposed to be such that no multiple collision can occur.

Given a lattice \(\mathcal{L}\), we consider that the spin \(\sigma\) (or angular momentum) of a particle takes only two possible values, say \(\sigma = \pm 1\). Then, depending on \(\mathcal{L}\), we can find \(\tau\) such that during \(\tau\) no molecule can undergo more than one collision (note that the supremum of such \(\tau\) does not verify this condition). The dynamics on \(\mathcal{L}\) define a dynamical system on the space \((\mathbb{T} \times \{-1, 1\})^2\), where \(\mathbb{T}\) is the one-dimensional torus. This is a continuous time dynamical system \((\mathbb{R}\) action) which is completely determined (with no significant loss of information) by its 1-time maps, provided the chosen time interval is some \(\tau\) as previously defined. The full initial dynamical problem is then reduced to the study of a diffeomorphism of \((\mathbb{T} \times \{-1, 1\})^2\). This is in fact a very difficult problem but we are now in a position to introduce probability into the problem. The justification for this is the diffusive character of the results obtained for the AMACF in 1-dimension in a molecular dynamic experiment.

This leads us to consider the following random walk. We start at time \(t = 0\) at site \(X = 0\) with a given value of \(\sigma \in \{-1, 1\}\). We then consider that collision events take place at discrete times \(t_i = n_i \tau\). It is to be noticed that this assumption is not an idealization: it represents fairly the initial dynamical system where the interaction had to be performed between \((n_i-1)\) and \(n_i\). At each step \(t = n_i\), we have a given constant probability \(p' = p/2\) for the collision of the rotator at site zero with one of its allowed neighbours, and a complementary probability \(q\) of no collision. The first collision therefore takes place at time \(t_1 = n_1\) \(\tau\) \((n_1\) not necessarily equal to 1). This collision produces the exchange and sign reversal of the spins of the rotator at site 0 with the rotator at some site \(X_1\). Next, we consider the interaction of the rotator at site \(X_1\) with its neighbourhood, etc.

Now comes the probabilistic modelling: we suppose the independence of successive events so that the successive steps of the process are those of a classical random walk on the lattice \(\mathcal{L}\) where the spin carried by the walker at time \(t = n\tau\) is equal to \((-1)^m\), where \(m\) is the total number of collisions performed by the walker at time \(t\).

4. Random walks with sign reversal : computation of the angular momentum autocorrelation function. — For the probabilistic models defined in the preceding section, there exists a well definite probability \(P_{n,s}(M)\) for the walker to be in site \(M\) at time \(t = n\tau\) after \(s\) collisions [6]. The time autocorrelation of spins will be defined by:

\[F_{\omega}(t) \equiv G(n) = \sum_{s=0}^{n} (-1)^s P_{n,s}(0).\]

Let us now consider the characteristic function of...
the probability law of the displacements over the lattice. Let $\langle e^{iM \cdot \Phi} \rangle_n$ be the expectation value at time $t = nr$ of $e^{iM \cdot \Phi}$ where $M = (m_1, m_2, ..., m_d)$ is the displacement vector on the $d$-dimensional lattice and $\Phi = (\varphi_1, \varphi_2, ..., \varphi_d)$ is a $d$-vector. $\langle e^{iM \cdot \Phi} \rangle_n$ can be put into the form:

$$\langle e^{iM \cdot \Phi} \rangle_n = [K(\{ \varphi_j \}) + q]^n,$$  

(3)

where the function $K(\{ \varphi_j \})$ depends on $\mathcal{C}$. Using the binomial expansion, equation (3) reads

$$\langle e^{iM \cdot \Phi} \rangle_n = \sum_{s=0}^{n} C_n^s K^s q^{n-s},$$  

(4)

where any term $C_n^s K^s q^{n-s}$ is obviously the contribution to $\langle e^{iM \cdot \Phi} \rangle_n$ of the $s$-collisions paths. Therefore, we have:

$$P_{n,s}(M) = \frac{1}{(2 \pi)^d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d\varphi_1 \cdots d\varphi_d \times$$

$$e^{-iM \cdot \Phi} C_n^s K^s q^{n-s},$$  

(5)

from which we obtain the autocorrelation function:

$$F_w(t) \equiv G(n) = \frac{1}{(2 \pi)^d} \times$$

$$\int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d\varphi_1 \cdots d\varphi_d \sum_{s=0}^{n} (-1)^s C_n^s K^s q^{n-s},$$  

(6)

or:

$$F_w(t) = \frac{1}{(2 \pi)^d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} [q - K(\{ \varphi_j \})] d\varphi_1 \cdots d\varphi_d.$$  

(7)

We see that, in the case of even lattices, $F_w(t)$ reduces to the probability $P_{n}(0)$ that the walker comes back to its initial position at time $t = nr$. We have thus a classical problem of random walk [6] on a lattice and we know that $P_n(0) \sim \frac{1}{n^{d/2}}$.

As an example, for the $d$-dimensional hypercubic lattice with $q = 0$, one finds

$$P_{2n}(0) \sim 2 \left( \frac{d}{4 \pi n} \right)^{d/2},$$

$$P_{2n+1}(0) \equiv 0$$  

(8)

and

$$P_{d}(0) \sim \left( \frac{d}{2(1 - q) \pi n} \right)^{d/2}$$  

(9)

when $q \neq 0$.

Let us now come to the case of odd lattices where typical effects of sign reversal first appear. We first consider a bidimensional triangular lattice which

The asymptotic evaluation of integral (7) shows (see Appendix A) that the integrand $Z = [q - K(\varphi_1, \varphi_2)]^n$ exhibits two maxima, namely $Z = 1 - 3 p'$ and $Z = 12 p' - 1$, which yield respectively the large $n$ value of the integral according to the value of $p = 2 p'$. We obtain:

$$F_w(t) \equiv G(n) = \frac{(1 - 3 p')^{n+1}}{4 \pi^{1/2} \sqrt{n}} 0 < p' < \frac{2}{15},$$

(12)

$$F_w(t) \equiv G(n) = \frac{(-1)^n (12 p' - 1)^{n+1}}{4 \pi^{1/2} \sqrt{n}} \frac{2}{15} < p' < \frac{1}{6}.$$  

(13)

Let us now consider a tridimensional lattice. It is easily seen that the cubic face centred lattice yields odd closed paths when interactions are allowed with (and only with) all nearest neighbours. Each particle has 12 nearest neighbours which are located at the middle of the edges of a cube whose centre is the site of the reference particle. Two odd closed paths are shown on figure 3.

Using the reference frame of figure 3, we obviously have:

$$K(\varphi_1, \varphi_2, \varphi_3) = 4 p' [\cos \varphi_1 \cos \varphi_2 + \cos \varphi_2 \cos \varphi_3 + \cos \varphi_3 \cos \varphi_1],$$  

(14)

with:

$$q + 12 p' = 1.$$  

(15)

Again, we find for $F_w(t)$ two different expressions according to the value of $p'$ (see Appendix B):

$$F_w(t) \equiv G(n) = \frac{(-1)^n (12 p' - 1)^{n+3/2}}{(2 \pi n p')} \frac{1}{8} < p' < \frac{1}{6},$$  

(16)
Fig. 3. Coordinate frame for the c.f.c. lattice. Two possible odd closed paths have been represented.

\[ F_w(t) \equiv G(n) < C(1 - 4p')^{n+1} \quad 0 < p' < \frac{1}{8} \]  

In these two examples, we find evidently that, for \( q = 0 \) (zero probability of no collision), \( |G(n)| \) decays as \( n^{-d/2} \) like \( P(n) \) in the usual random walk. On the contrary \( |G(n)| \) has an exponential decay when \( q \neq 0 \). Further numerical investigations on various lattices lead us to think that this feature is quite general. We also remark that, for small enough \( q \) values, the decay is oscillatory \( (G(n) \) taking successively positive and negative values) whereas this evolution is monotonic for larger \( q \) values.

We shall end this section by describing some semi-qualitative results on the intermediate time behaviour of \( F_w(t) \) for odd lattices with \( q \neq 0 \).

We have done a great number of numerical computations, varying \( q \) in the domain of monotonic asymptotic exponential decay of the AMACF and using different kinds of odd lattices.

In each case, for intermediate time (roughly up to \( n = 20 \)), we observed behaviours which fitted some \( at^{-3} - b \) law with a \( 10^{-3}\) error (see the examples given on figure 4).

This intermediate behaviour is to be compared to the same type of \( at^{-3} - b \) law that appeared as pre-asymptotic behaviour of the angular momentum autocorrelation function in 2-d diatomic Lennard-Jones fluids. This coincidence seems to confirm that this behaviour, when observed in 2-d fluids, may be related to the cog-wheel mechanism which can arise in a liquid, due to the existence of a local order [7] which, by its very imperfect character, will generally contain many odd-type local structures. At this point, it is worth noting that some \( at^{-3} - b \) pre-asymptotic behaviours exist also in the numerical experiments reported in [2] on quite different ellipsoidal molecules but not in rough disks: in the latter model no local plastic crystals can indeed exist.

5. Numerical molecular dynamic simulations on lattices of diatomics. — We now focus our attention on more realistic models of plastic crystals, namely assemblies of diatomic molecules interacting via the truncated Lennard-Jones diatomic potential used in previous simulations of 2-d liquids [3, 4]. We used lattices of 1600 molecules with periodic boundary conditions. In order to have the best observations of the long time behaviour of the AMACF, we choose the lattice translation in such a way that the potential energy during a collision was of the same order of magnitude as the mean kinetic energy.

This prevents the AMACF from exhibiting a series of negative overshoots at short times, a feature which would indicate that the rotational motions predominantly have the form of librations rather than rotations. Except for the simplifications due to the existence of a lattice (no translation motion; the neighbours of each molecule are always the same ones) the computations were done as for 2-d fluids; we refer to reference [3, 4] for more details.

Note that for such models, the total angular momentum is not conserved (due to the reaction of the pivots, as noted above). (However, we observed that it is conserved when averaged over time). Even the sum of the norms of the individual angular momenta of the molecules is not conserved, due to the violation of (1). (At this point, let us point out that the lattice
translation and the range of the interacting potential were chosen in such a way that the pseudo collisions were not too different from eq. (1). The unique integral of motion seems thus to be the total energy of the system.

We now present the result of numerical experiments using both the square and the triangular lattices. In the square (even) lattice, we observed (Fig. 5) instead of the decay

\[ F_w(t) \propto \frac{a}{t} \quad (t \text{ large}) \quad (18) \]

which is predicted by the random walk model, a \( \frac{a}{t} - b \) decay, where \(-b\) might be associated with the non-conservation of the norms of individual angular velocities. For the triangular lattice, after 40 000 steps of the numerical algorithm, the results presented fluctuations (when comparing 10 000 steps runs) that indicate a prohibitive cost for reliable results. At least one can say that these incomplete results are compatible (Fig. 6) both with the \( at^{-3} - b \) presasymptotic behaviour already observed in liquids (see also the end of section 4), and at longer times with the fast asymptotic decay predicted by random walk models.

6. Summary and conclusion. — In order to study the long time behaviour of the angular momentum autocorrelation function \( F_w(t) \) in rotatory (plastic) crystals, we have introduced a classification into odd and even lattices depending on whether or not the information given by a molecule to a neighbour during a collision can come back to its initial site after an odd number of collisions. We propose a model of random walks which allows us to obtain typically different results for \( F_w(t) \), according to the parity of the lattice. The validity of this Markovian model seems to be confirmed, at least in one dimension and for a square lattice. Some related observations confirm the conjecture previously put forward on the relevance of cog-wheel mechanism for intermediate time behaviours of the angular momentum correlation functions in 2-d fluids at intermediate densities. More generally, the asymptotic exponential decay of the AMACF in many body systems whose particles can exchange spin angular momentum would be a valuable result with interesting consequences in kinetic theory. However, we emphasize that this behaviour has been proved in this paper only in the frame work of the random walk model. This model is based on the statistical independence of successive collision events. Therefore, it would be interesting to perform Molecular Dynamics calculations (e.g. on the triangular lattice) with hard core particles, and to get better statistics than we succeeded in obtaining with soft core (Lennard-Jones) ones.

**APPENDIX**

A. Bidimensional triangular lattice.

\[ K(\varphi_1, \varphi_2) = \frac{P}{2} \left[ \cos \varphi_1 + \cos \varphi_2 + \cos (\varphi_1 - \varphi_2) \right] \]

with \( 3p + q = 1 \quad (0 < p < \frac{1}{3}) \)
and
\[ G(n) = \frac{1}{4 \pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \times \{ q - p(\cos \varphi_1 + \cos \varphi_2 + \cos (\varphi_1 - \varphi_2)) \}^n d\varphi_1 d\varphi_2. \]

Changing the variables
\[ \varphi_1 = x + y \]
\[ \varphi_2 = x - y \]
we have :
\[ G(n) = \frac{1}{4 \pi^2} \times \int \int_{(c)} \{ 1 - 2p - 2p(\cos x \cos y + \cos^2 y) \}^n dx dy \]

the integration domain (c) is the square with corners
\((\pi, 0); (0, \pi); (-\pi, 0); (0, -\pi)\). The extrema of
\[ Z(y) = 1 - 2p - 2p(\cos x \cos y + \cos^2 y) \]
are defined by
\[ \sin x \cos y = 0 \]
\[ \sin y(\cos x + 2 \cos y) = 0 \]
which relations yield the following points
1) \[ \sin x = 0 \rightarrow \{ x = 0 \}
\sin y = 0 \rightarrow \{ y = 0 \} \quad (Z = 1 - 6p) \]
2) \[ \cos x = \cos y = 0 \rightarrow Z = 1 - 2p \]
3) \[ \sin x = 0 \rightarrow \{ Z = 1 - \frac{3p}{2} \}
\cos y = \pm \frac{1}{2} \rightarrow \{ Z = 1 - \frac{7p}{2} \}.
\]
Since \(0 < p < \frac{1}{3}\) we always have
\[ \left| 1 - \frac{3p}{2} \right| > \left| 1 - 2p \right|, \]
therefore the contribution of the extremum
\[ \cos x = \cos y = 0 \]
is negligible, compared with those of
\[ \{ \sin x = 0, \cos y = \pm \frac{1}{2} \}. \]
Now, if \(p\) is such that \(1 - \frac{7p}{2} > 0\), then
\[ 1 - \frac{7p}{2} < 1 - \frac{3p}{2}. \]
If \(1 - \frac{7p}{2} < 0\), then \(1 - 6p\) is greater than \(1 - \frac{7p}{2}\). This shows that the dominant contributions to the integral for large \(n\) are given by \((x, y)\) points for which
\[ Z = 1 - \frac{3p}{2} \quad \text{or} \quad Z = 1 - 6p. \]
These points (lying in the integration domain (c)) are :
\[ A_0 \begin{cases} x = 0 \\ y = 0 \end{cases} \rightarrow Z = 1 - 6p \]
\[ A_1 \begin{cases} x = 0 \\ y = \pm \frac{2\pi}{3} \end{cases} \rightarrow Z = 1 - \frac{3p}{2} \]
the last two points giving obviously equal contributions. As we shall see, these points yield contributions respectively proportional to \((6p - 1)^{n+1}\) and
\[ \left(1 - \frac{3p}{2}\right)^{n+1}. \]
Therefore, these contributions are dominant in different adjacent \(p\) domains separated by the value \(p_0\) such that \(6p_0 - 1 = 1 - \frac{3p_0}{2}\), namely \(p_0 = \frac{4}{15}\).

Case 1 : \(\frac{4}{15} < p < \frac{1}{3}\).

The large \(n\) value of the integral is given by the neighbourhood of \(A_0(x = 0, y = 0)\). Expanding \(Z\) around \(A_0\) gives :
\[ Z = 1 - 6p + p(x^2 + 3y^2) \]
and
\[ G_\infty(n) = \frac{(-1)^n}{2\pi^2} (6p - 1)^n \times \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \exp\left[-\frac{np}{6p - 1}(x^2 + 3y^2)\right] dx dy \]
where \(G_\infty(n)\) means \(\lim_{n \to \infty} G(n)\). We finally obtain
\[ G_\infty(n) = \frac{(-1)^n (6p - 1)^{n+1}}{2\pi\sqrt{3}} \cdot \frac{2}{p} \]
\[ Case 2 : x = 0, y = \pm \frac{2\pi}{3}. \]
Expanding \(Z\) around any one of these points, gives :
\[ Z = 1 - \frac{3p}{2} - \frac{p}{2}(x^2 + 3y^2). \]
\[ \left(\text{where } v = y + \frac{2\pi}{3}\right). \]
Summing the equal contributions of $A_+$ and $A_-$, we obtain:

$$G_{\infty}(n) = \frac{1}{\pi^2} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx \, dy \times$$

$$\times \left\{ 1 - \frac{3 \rho}{2} - \frac{\rho}{2} (x^2 + 3 y^2) \right\}^n,$$

which yields

$$G_{\infty}(n) = \frac{2}{\pi^{3/2}} \left( 1 - \frac{3 \rho}{2} \right)^{n+1} \frac{1}{\rho n}.$$

B. Three-dimensional c.f.c. lattice. — Using the expression given for $K(\varphi_1, \varphi_2, \varphi_3)$ in the main text, $G(n)$ reads

$$G(n) = \frac{1}{\pi^3} \int_{0}^{\pi} \int_{0}^{\pi} \int_{0}^{\pi} \{ 1 - 3 \rho - \rho \cos \varphi_1 \cos \varphi_2 +$$

$$+ \cos \varphi_2 \cos \varphi_3 + \cos \varphi_3 \cos \varphi_1 \} \rho^2 d\varphi_1 \, d\varphi_2 \, d\varphi_3$$

$$\quad (0 < \rho < \frac{1}{3})$$

(the integration domain has been reduced to a cube in the positive space, owing to the symmetry properties of the integrand). Introducing

$$Z = 1 - 3 \rho - \rho n \cos \varphi_1 \cos \varphi_j,$$

the extrema of $Z$ obey the relations

$$\begin{align*}
\sin \varphi_1 (\cos \varphi_2 + \cos \varphi_3) &= 0 \\
\sin \varphi_2 (\cos \varphi_3 + \cos \varphi_1) &= 0 \\
\sin \varphi_3 (\cos \varphi_1 + \cos \varphi_2) &= 0
\end{align*}$$

the largest extrema are given by

$$\begin{align*}
\varphi_1 &= \varphi_2 = \varphi_3 = 0 \\
\varphi_1 &= \varphi_2 = \varphi_3 = \pi
\end{align*}$$

giving $Z = 1 - 6 \rho$ (these two points yielding equal contributions to $G(n)$).

2) Points such that $\cos \varphi_1 = \cos \varphi_2 = \cos \varphi_3 = 0$. These points yield $Z = 1 - 2 \rho$. $Z = 1 - 2 \rho = 6 \rho - 1$ for $\rho = \frac{1}{4}$. It is easily seen that the contributions of points 3) are always dominated by those of points 1) or points 2). Indeed we have:

$$\begin{align*}
\rho_1 &= 0 \quad \rho_2 = \pi \quad \rho_3 \text{ arbitrary} \\
\rho_1 &= 0 \quad \rho_3 = \pi \quad \rho_2 \text{ arbitrary} \\
\rho_2 &= 0 \quad \rho_1 = \pi \quad \rho_3 \text{ arbitrary} \\
\rho_2 &= 0 \quad \rho_3 = \pi \quad \rho_1 \text{ arbitrary}
\end{align*}$$

giving $Z = 1 - 2 \rho$.

3) Points such that $\cos \varphi_1 = \cos \varphi_2 = \cos \varphi_3 = 0$. These points yield $Z = 1 - 3 \rho$. $Z = 1 - 3 \rho = 6 \rho - 1$ for $\rho = \frac{1}{4}$. It is easily seen that the contributions of points 3) are always dominated by those of points 1) or points 2). Indeed we have:

$$\begin{align*}
\rho_1 &= 0 \quad \rho_2 = \pi \quad \rho_3 \text{ arbitrary} \\
\rho_1 &= 0 \quad \rho_3 = \pi \quad \rho_2 \text{ arbitrary} \\
\rho_2 &= 0 \quad \rho_1 = \pi \quad \rho_3 \text{ arbitrary} \\
\rho_2 &= 0 \quad \rho_3 = \pi \quad \rho_1 \text{ arbitrary}
\end{align*}$$

giving $Z = 1 - 2 \rho$. $Z = 1 - 2 \rho = 6 \rho - 1$ for $\rho = \frac{1}{4}$. It is easily seen that the contributions of points 3) are always dominated by those of points 1) or points 2). Indeed we have:

$$\begin{align*}
\rho_1 &= 0 \quad \rho_2 = \pi \quad \rho_3 \text{ arbitrary} \\
\rho_1 &= 0 \quad \rho_3 = \pi \quad \rho_2 \text{ arbitrary} \\
\rho_2 &= 0 \quad \rho_1 = \pi \quad \rho_3 \text{ arbitrary} \\
\rho_2 &= 0 \quad \rho_3 = \pi \quad \rho_1 \text{ arbitrary}
\end{align*}$$

giving $Z = 1 - 2 \rho$.

Case 1 : $0 < \rho < \frac{1}{4}$.

Evaluating the asymptotic contribution of the neighbourhood of extremal lines is a rather delicate problem, and we shall only give an upper bound of this evaluation, which does confirm that $G(n)$ has at least an exponential decay.

Let us consider the line $[\varphi_2 = 0, \varphi_1 = \pi]$, and put $\varphi_1 = \pi - u, \varphi_2 = \varphi, \varphi_3 = \pi - v$. We obtain

$$Z = 1 - 2 \rho - 4 \rho \left\{ \sin^2 \frac{\varphi}{2} \left[ 1 - \left( \sin^2 \frac{u}{2} + \sin^2 \frac{v}{2} \right) \right] \right\}$$

which leads to an asymptotic contribution to $G(n)$ of the form:

$$A(n) = \frac{(1 - 2 \rho)^n}{\pi^3} \int_{0}^{\pi} \int_{0}^{\pi} \int_{0}^{\pi} \exp \left\{ - \frac{4 \rho n}{1 - 2 \rho} \left[ \sin^2 \frac{\varphi}{2} \left( 1 - \left( \sin^2 \frac{u}{2} + \sin^2 \frac{v}{2} \right) \right) + \sin^2 \frac{u}{2} \sin^2 \frac{v}{2} \right] \right\} \, d\varphi \, du \, dv.$$

Integrating over $\varphi$ the integrand peaked around $\varphi = 0$ yields

$$A(n) = \frac{\pi^{-5/2}}{2} \frac{(1 - 2 \rho)^n \sqrt{n}}{\sqrt{np}} \int_{0}^{\pi} \int_{0}^{\pi} \frac{du \, dv}{\sqrt{1 - \left( \sin^2 \frac{u}{2} + \sin^2 \frac{v}{2} \right)}} \exp \left\{ - \frac{4 \rho n}{1 - 2 \rho} \sin^2 \frac{u}{2} \sin^2 \frac{v}{2} \right\}.$$
Making the change of variables \((\sin \frac{u}{2}, \sin \frac{v}{2}) \rightarrow (x, y)\), the double integral reads:

\[
\int_0^1 \int_0^1 dx \, dy \phi(x, y) \exp\left( -\frac{4}{1-2p} x^2 y^2 \right)
\]

where \(\phi(x, y)\) is an integrable function over the \((x, y)\) domain of integration (this is easily verified).

Let

\[
 J = \int_0^1 \int_0^1 \phi(x, y) \, dx \, dy
\]

we have, summing up the equal contributions of the six lines,

\[
 G(n) < 3 \pi^{-5/2} \left( 1 - 2p \right)^{n+\frac{3}{2}} B(n)
\]

with

\[
 B(n) = J \int_0^1 \int_0^1 \exp\left( -\frac{4}{1-2p} x^2 y^2 \right) \, dx \, dy.
\]

Integrating the last integral over \(y\), we obtain:

\[
 B(n) = J \int_0^1 \left[ \exp\left( -\frac{4}{1-2p} x^2 \right) \right] \, dx \, dt
\]

where

\[
 \text{Erf}(z) = \int_0^z e^{-t^2} \, dt
\]

whose asymptotic limit is

\[
 B(n) \rightarrow \frac{J}{2} \sqrt{\frac{1-2p}{pn}} \frac{\sqrt{\pi}}{2} \ln \left[ 2 \frac{\sqrt{\frac{pn}{1-2p}}} {\sqrt{\frac{1-2p}{pn}}} \right] \rightarrow \frac{\sqrt{\pi}}{8} \frac{J}{\sqrt{1-2p}} \ln (n).
\]

Therefore, we conclude that, for large \(n\)

\[
 G(n) < \frac{3J}{8 \pi^2} \left( 1 - 2p \right)^{n+1} \ln (n) < \frac{3J}{8 \pi^2} \left( 1 - 2p \right)^{n+1}.
\]

Of course \(G(n)\) is not oscillatory.

Case 2: \(\frac{1}{4} < p < \frac{3}{4}\).

The contribution due to points \((0, 0, 0)\) and \((\pi, \pi, \pi)\) are calculated without difficulty, as in the case of the triangular lattice. We obtain

\[
 G_{\infty}(n) = \frac{(-1)^n}{4} \frac{(6p - 1)^{n+\frac{3}{2}}}{(\pi np)^3}.
\]

References
