On the most compact regular lattices in large dimensions

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In this talk I will consider the computation of the maximum density of regular lattices in large dimensions using an approach based on statistical mechanics.

The starting point will be some theorems of Rogers, which are virtually unknown in the community of physicists.

Using his approach one can find many similarities (and differences) with the problem of computing the entropy of a system of hard spheres. The relation between the two problems is investigated in detail. Some conjectures are presented: further investigation is needed in order to check their consistency.

Which is the maximum density of hard spheres when they are packed on a regular lattice? In two and three dimensions the solution is well known; the lattices with maximal packing density are the hexagonal and the ffc lattices respectively.

In generic dimensions the result for the maximal packing density in not known: a lower bound on the maximal packing density has been established by Minkowski. We are interested to the infinite dimension limit.

We will introduce the Rogers measure over the space of all possible lattices.
We will show how to compute the moments of a function of the lattice using the Rogers I will present some simple computations in order to become more familiar with Rogers results.
Finally in the last section we start a comparison between the packing problem and the thermodynamic of hard spheres; I present a conjecture for the relation between these two problems in the infinite dimension limit.

How to parametrize the lattice?

To each matrix unimodular matrix Λ of this set we can associate a regular lattice, having cells of unit volume, that is given by all the points of the form

$$x_i = \sum_k \Lambda_{i,k} n_k \equiv (\Lambda n)_i,$$

where the n_k take all the possible integer values (both positive and negative). This correspondence is not one to one

If we consider non overlapping spheres centered on the points of the lattices, the maximum allowed *diameter* ($\mathcal{R}(\Lambda)$) is given by

$$\mathcal{R}(\Lambda)^2 = \min_n |\Lambda n|^2$$

and the minimum is done over all the possible choices of the integer D-dimensional vector n, with the exclusion of the origin. Our aim is to compute

$$\mathcal{R}_M = \max_\Lambda \mathcal{R}(\Lambda).$$

The computation of the minimum for generic Λ is an NP-hard problem for large dimensions D.

We introduce the notation

$$\langle f(|x|)\rangle_\Lambda \equiv \sum_n f(|x(n)|) \equiv \sum_n f(|\Lambda n|),$$

where the sum is done over Z^D, origin excluded.

$$\mathcal{R}(\Lambda)^2 = -\lim_{\beta\to\infty} \ln(F(\beta)_\Lambda,) \qquad F(\beta)_\Lambda = \frac{\langle \exp(-\beta|x|^2)\rangle_\Lambda}{\beta}.$$

In other words $|x|^2$ is the Hamiltonian,

$$Z(\beta)_\Lambda \equiv \langle \exp(-\beta|x|^2)\rangle_\Lambda$$

is the partition function and $\mathcal{R}(\Lambda)^2$ is the ground state energy.

The maximum packing density problem is a minimax problem, i.e. it consists in finding the matrix Λ such the ground state energy is as large as possible.

Alternatively we consider the quantity

$$K(R)_\Lambda = \langle \theta(R - |x|)\rangle_\Lambda,$$

$$K(R)_\Lambda = 0 \quad \text{for} \quad R < \mathcal{R}(\Lambda), \qquad K(R)_\Lambda > 0 \quad \text{for} \quad R > \mathcal{R}(\Lambda).$$

In order to formulate the statistical problem we must firstly introduce a measure $d\mu(\Lambda)$ on the space of all possible lattices.

$$\overline{F(\Lambda)} = \int d\mu(\Lambda) F(\Lambda).$$

If the measure $d\mu(\Lambda)$ does not vanish near the maximum of $\mathcal{R}(\Lambda)$, we can extract the value of $\mathcal{R}_M$ from the properties of the appropriate averages.

We can compute the moments of $K(R)_\Lambda$:

$$K^{(s)} = \overline{K(R)^s_\Lambda} \equiv \sum_{k=0,\infty} P(k,R) k^s \ .$$

The function $P(k,R)$ is the probability that a lattice has k points inside a sphere of radius R.

When $R > \mathcal{R}_M$ there are no lattices with no points inside a sphere of radius R. It is evident that

$$P(0,R) > 0 \quad \text{for} \quad R < \mathcal{R}_M, P(0,R) = 0 \quad \text{for} \quad R > \mathcal{R}_M.$$

The program consists in reconstructing the function $P(k,R)$ from its moments: in this way one can find the value of $\mathcal{R}_M$.

We must chose the measure $d\mu(\Lambda)$.

There is a natural definition (due to Siegel) of the measure over unimodular matrices, restricted to the fundamental region, each lattice may be represented in one and only one way by a matrix in the fundamental region.

We can consider the set of matrices Λ (introduced by Rogers) that at fixed ω depend on $D-1$ α-variables. The action of such a matrix on a vector is defined as

$$(\Lambda n)_i = \omega n_i \quad \text{for} \quad i < D, (\Lambda n)_D = \eta \left(n_D + \sum_{i=1,D-1} \alpha_i n_i \right),$$

where the unimodularity condition implies that

$$\omega^{D-1} \eta = 1.$$

The ω-dependent measure is obtained by taking a flat measure in the interval 0-1 for each of the $D-1$ α-variables. Eventually the limit $\omega \to 0$ is taken.

The computations with the Rogers measure are much simpler. The two measures are equivalent for our purposes: the quantities

$$\overline{\langle f \rangle}^{s}_{\Lambda}$$

are the same if evaluated with the two measures.

The first result one can prove is:

$$\overline{\langle f \rangle}_{\Lambda} = \int d^D x f(x) \ .$$

If we apply this result to the case $f(x) = \theta(R - |x|)$ we find that

$$\overline{K(R)} \equiv \sum_{k=0,\infty} P(k,R)k = V_D(R) \ ,$$

where $V_D(R) \equiv R^D \pi^{D/2} \Gamma(D/2+1)^{-1}$ is the volume of the D-dimensional sphere of radius R. The function $K(R)_\Lambda$ may take only even integer values and consequently $P(0,R)$ must be different from zero in the region where

$$V_D(R) < 2,$$

that is also a consequence of the celebrated Minkowski theorem in large dimensions.

Let us call R_c the D-dependent value of R such that

$$V_D(R_c) = 1 \ .$$

It is convenient to measure all the lengths in units of R_c when the dimension D go to infinity. At this end we define:

$$r = R/R_c, \quad r_M = \mathcal{R}_M/R_c \ .$$

When the dimensions D go to infinity, we face the problem of finding the limit of r_M that we suppose to exist. The following bounds are known for infinite D:

$$1 \leq r_M \leq 1.322.$$

The lower bound is the Minkowski theorem, while the upper bound is the Kabatiansky-Levenshtein bound)

Rogers main theorem Let us recall some known results of the values of the moments of the function f,

$$\overline{f^s} \equiv \overline{\left(\sum_n f(\Lambda n) \right)^s} \ ,$$

in the case where $s < D$. We shall see later how this annoying constraint ($s < D$) may be removed.

$$\overline{f} \equiv \overline{\sum_n f(\Lambda n)} = \int_{-\infty}^{\infty} d^D x f(x) \ .$$

The strategy for computing the moments defined in eq. consists of a few steps:

- We classify all sets of s vectors n_k $(k = 1, \ldots s)$ according to their linear dependence.
- We perform the average and the sums inside each class.
- We write the final result the sum over all possible classes.

The crucial theorem is based on the following two lemmas.

$$\overline{\sum_{n^k}^{LI}\left(\prod_{k=1,s} f(\Lambda n^k)\right)} = \left(\int d^D x f(x)\right)^s ,$$

where $\sum^{LI}$ denotes the sum over all the sets of s vectors n^k belonging to Z^D that are linearly independent (as usual the origin, i.e. $n^k = 0$, never appears). The formula is valid only for $s \leq D$ and it has a very simple meaning. By changing the lattice each of the s points n^k may be carried in any point of the space independently from the other one, provided that they are linearly independent.

We introduce s vectors n that are linear combination of $s-h$ linear independent vectors and their linear dependence is specified by a matrix M. The s vectors n span a $(s-h)D$ dimensional space and they satisfy the following h (vectorial) linear conditions:

$$\sum_{k=1,s} M_{j,k} n^k = 0 \quad \text{for} \quad j = 1, h \ ,$$

where the matrix M has integer elements and it is irreducible (there is no integer matrix M' such that $pM' = M$ with p integer). The previous case corresponds to $h = 0$.

In this case we find that

$$\overline{\sum_{n_i^k}^{(M)} \left(\prod_{k=1,s} f(\Lambda n^k) \right)} = \mathcal{N}(M) \int \prod_{k=1,s} d^D x^k f(x^k) \prod_{j=1,h} \delta^D \left(\sum_{k=1,s} M_{j,k} x^k \right) \ ,$$

where the sum $(\sum^{(M)})$ is done on vectors that satisfy the condition (12) (they depend on the matrix M and have $s-h$ linear independent components). The quantity $\mathcal{N}(M)$ is a normalization factor that is equal to 1 in many cases; for our purposes it may be taken equal to 1.

We consider all possible linear dependence of the vectors n and we transform the sum over all the values of n to a sum over all possible linear dependencies. We can now state the main theorem of Rogers :

$$\overline{< f >^s} = \sum_{h=0,s-1} \sum_{M} \mathcal{N}(M) \int \prod_{k=1,s} d^D x^k f(x^k) \prod_{j=1,h} \delta^D \left(\sum_{k=1,s} M_{j,k} x^k \right) ,$$

where the sum is done over all the sets of $h \times s$ matrices M corresponding to different linear conditions.

The case $s = 2$

Here we have to compute

$$\overline{\sum_{n_1,n_2} f(n_1)f(n_2)} \, .$$

Now we have two possibilities:

- The two vectors n are linearly independent. We obtain the following contribution

$$\int d^D x_1 d^D x_2 f(x_1)f(x_2) \, .$$

- We consider the case where the two vectors n are linearly dependent. In this case we can write the constraint in an unique way as

$$q_1 n^1 + q_2 n^2 = 0 \, ,$$

if we restrict ourselves to the case of positive q_1 and $(q_1, q_2) = 1$ (i.e. the pair q_1 and q_2 is irreducible)

We finally finds the following contribution

$$\int d^D x d^D y f(x)f(y)\delta^D(q_1 x + q_2 y) = \int d^D x f(q_1 x)f(q_2 x).$$

Putting everything together we find the final expression

$$\overline{\sum_{n_1,n_2} f(n_1)f(n_2)} = \int d^D x_1 d^D x_2 f(x_1)f(x_2) + \sum_{q_1,q_2}^{I} \int d^D x f(q_1 x) f(q_2 x)\,,$$

where the sum $\sum^I$ is restricted over the irreducible pairs with q_1 positive.

The Gaussian case

Let us consider the case where the function $f(x)$ is given by

$$f(x) = (2\pi)^{-D/2} \exp(-\beta x^2/2).$$

Here the integrals can be easily done and we finds that

$$\overline{< f >} = \beta^{-D/2} \overline{< f^2 >} = \beta^{-D} + \beta^{-D/2} \sum_{q_1, q_2}^{I} (q_1^2 + q_2^2)^{-D/2} \ ,$$

For large D we find:

$$(\overline{< f >})^{-2/D} = \beta^{-1} \ , (\overline{< f >^2})^{-2/D} \approx \max(\beta^{-2}, (2\beta)^{-1}) \ ,$$

The problems connected with the limit $D \to \infty$ are clear from the previous formulae. Depending on the value of β different terms are the leading ones (the case $\beta < 1$, $1 < \beta < 2$, $2 < \beta$ are different).

The terms with the q's and the g's equal to 1 are always the leading ones inside a given class.

Summing the leading terms

Generalizing the analysis of the first moments one concludes that at given value of h the leading terms, when the dimensions go to infinity, come from h linear conditions of the form

$$\sum q_i x_i = 0$$

with $q_i \in \pm 1$.

If we select these contributions the result can be given in terms of h integrals of the same function. We get:

$$\overline{< f >^s} \approx \sum_{h=1,s} \prod_{i=1,h} \left(\sum_{\nu_i=1,s} C(s,h,\nu) 2^{\nu_i - 1} \int d^D x f(x)^{\nu_i} \right) ,$$

where the sum is done over all the sets of h integers ν_i such that

$$\sum_i \nu_i = s,$$

and $C(s,h,\nu)$ is a combinatorial factor.

After some simple algebra we find that

$$\overline{\exp(y < f >)} \approx \exp\left(\frac{1}{2}\int dx(\exp(2yf(x)) - 1)\right) \ .$$

If we apply this formula to the case of the theta function we find that

$$\overline{\exp(yK(R)_\Lambda)} \approx \exp\left(\frac{V_D(R)}{2}(\exp(2y) - 1)\right) = \exp\left(-\frac{V_D(R)}{2}\right) \sum_{k=0,\infty} \frac{1}{k!}\left(\frac{V_D(R)}{2}\right)^k \exp(2ky) \ .$$

At the end we get a simple result:

$$P(2k, R) \approx \exp\left(\frac{-V_D(R)}{2}\right) \frac{1}{k!}\left(\frac{V_D(R)}{2}\right)^k \ ,$$

while $P(2k+1, R) = 0$ (The number of points of a lattice inside a sphere is always even!).

This Poisson distribution implies that

$$P(0, R) \approx \exp\left(\frac{-V_D(R)}{2}\right) \ .$$

R_c is the radius of a sphere of unit volume. If we take a large value of D at fixed ratio $r \equiv (R/R_c)\ V(rR_c)$ goes to zero or to infinity depending if r is smaller or greater than 1.

- If $r < 1$, $P(0, rR_c)$ goes to 1 apart from exponentially small corrections. With probability going to 1 lattices do not have points at distance smaller that R_c.
- In the interesting case $r > 1$ this computation give an exponentially small, but non-vanishing, contribution for $P(0, rR_c)$.

$P(0, rR_c)$ is always non zero and we can find always a lattice that contains no points at distance less than rR_c. This result cannot be correct because it can be proved that no such lattice exist for large D as soon $r > 1.322$.

This failure arise from neglecting exponentially small terms. We cannot neglect the subleading terms if there are strong cancellations among the leading terms and if the sum of the leading terms becomes smaller of some subleading term. It was proved by Rogers that these cancellations do not happen in the relatively small region where $r^D < D$ and this leads to a marginal improvement of the Minkowski bound.

The importance of being connected

Let us consider an integer valued function f and its moments defined as

$$< f^s >= \sum_k P(k) k^s = \sum_G \int \prod_{i=1,n} (d^D x_i f(x_i)) G(\{x\}) \ ,$$

where the sum is done over the appropriate set of function $G(\{x\})$. These functions are an appropriate product of delta functions that enforce the linear dependence of some of the x's.

A function G is connected if it goes to zero when one or more of the x go to infinity together.

If G is not connected, it can be written as the product of its connected pieces. If we take care of all the multiplicity factors and we use the standard manipulations of statistical mechanics we find that

$$< f^s >_c = \sum_{G_c} \int \prod_{i=1,n} \left(d^D x_i f(x_i) \right) G_c(\{x\}) \, ,$$

where the sum is done only over those G that are connected (we call them $G_c(\{x\})$).

A new difficult

The program we have put forward may seem witless.

We can write an equation) of the form

$$\overline{f^s} = F(s, D)\,,$$

that is valid only for $s < D$: for $s \geq D$ for the very good reason that in this case both sides of equation are infinite.

How could we write a meaningfully expression in finite dimension for $\overline{\exp(y < f >}$, if we can compute only a few moments of the $< f >$?

I would like to put forward a reasonable conjecture that should allow us to overcome this difficulty.

A preliminary conjecture We conjecture that each given moment can be computed at sufficient high dimensions, where it is convergent, and that we can evaluate it as analytic continuation in D and s at the point we need it.

The analytic continuation of the moments in the dimensions D at fixed s and the analytic continuation of the moments in the value of s at fixed dimensions D should coincide.

If this conjectures are true, Rogers formulae bring information on the function $P(k)$ also in the region where its moments are divergent: our program make sense.

I do not know how these conjectures could be proved in a rigorous and systematic way. One could in principle check by explicit computations that the leading singularities at $z = 0$ (or equivalently the tails of the function $P(k)$ at large k) are correctly reproduced.

The statistical mechanics of hard spheres

Let us consider the partition function of a system of hard spheres of diameter R at density 1:

$$Z(\mathcal{V}, N) = \int \prod_{i=1,N} dx_i \prod_{i,k=1,N} \theta(|x_i - x_k| - R) \ .$$

$$Z(\mathcal{V}, N) \approx \exp(\mathcal{V}\ S_H(r)) \ ,$$

where $S_H(r)$ is the entropy density of hard spheres and r is the reduced diameter.

The entropy should diverge when $r = r_A$, i.e. the highest density packing.

We do not know if the highest density packing is a lattice packing and if $r_A = r_M$.

In dimensions 3 the most compact packing is a lattice packing and $r_A = r_M$. Therefore the partition function vanishes as soon as $r > r_M$ and

$$\lim_{r \to (r_M)^-} S_H(r) = -\infty \, .$$

In three dimensions hard sphere crystallize: there is a diameter r_C such that for $r > r_C$ the configurations of the hard particles are very similar to those of a regular crystal.

Generally speaking in higher dimensions we can have two possibilities:

1. The partition function of hard spheres is different from zero also in the region $r > r_M$ and diverges at a value of $r = r_A > r_M$.
2. As in the three dimensional case the partition function of hard spheres becomes zero at $r_M = r_A$. We can however distinguish among two cases.
   (a) There is a diameter r_C where the entropy has a singularity and the system crystallize.
   (b) There is no crystallization transition.

We consider also the possibility of having a glass transition in the non-crystalline phase at the point r_G. This glass transition may be or in the metastable phase above r_C, as in three dimensions, or in the stable liquid phase below r_C. This glass phase transition is important because the virial expansion does not give information on the behaviour above r_G. There are arguments that predict that $r_G = 1$.

A first look to the virial expansion

Our aim is to compare the virial expansion for the partition function with the formulae that we have obtained for $\ln(P(0,r))$. Let us consider firstly the results that we obtain if we consider a particular class of diagrams, i.e. those of a chain. In this case one finds that

$$-S_H(r) = V(R) + \sum_{k=3,\infty} k^{-1} \int \prod_{i=1,k} d\nu(x_i) \delta \left(\sum_{i=1,k} x_i \right) \ ,$$

$$d\nu(x) = d^D x \theta(R-x) \ .$$

We would like to compare this result with the homologous one for the quantity $S_L(r) \equiv \ln(P(0,r))$.

One finds, among many other terms the following terms

$$-S_L(r) = V(R) + \sum_{k=2,\infty} \int \prod_{i=1,k} \left(d\nu(x_i) \sum_{q_i} \right) \delta \left(\sum_{i=1,k} x_i q_i \right) \ ,$$

where the sum over the q is done with the condition:

- All q are different from zero.
- Conventionally q_1 is positive.
- The set of k variables q_i for $i = 1, k$ is irreducible, i.e. they do not have common factors.
- For $k = 2$ the terms with $q_1 = 1 = \pm q_2$ are absent.

At each given k the leading term in the sum comes from those term where $q_1 = 1$ and $q_i = \pm 1$. If we retain only these contributions, we find (neglecting factors two) exactly the same result that for the $S_H(r)$.

The expression for $S_L(r)$ coincide with that for $S_H(r)$ obtained summing a subset of diagrams of the virial expansion.

This result can be simply understood: the distribution of the points of a random lattice are random if they do not satisfies linear constraints.

A more refined conjecture and open problems

- $S_H(r)$ is the entropy for a gas of hard spheres as function of the diameter. It may have singularities at various values of r.
- $S_L(r) = \ln(P(0, r)$, i.e. the logarithm of the probability of finding a lattice packing with reduced radius r. It should diverge toward infinity when we reach the maximum density for a lattice packing, i.e. r_M. This function can be written as an integral over a finite dimensional space so for fixed D it should be a smooth function of the radius. Only in the infinite dimensions it could develop a real first order phase transition, however it could be possible to observe the premonitory signs of this transition by evaluating it numerically. It is also not clear if a glass transition at $r = 1$ is present also for this function.
- $S_I(r)$ The two previous quantities are not easy to compute. One could use here a third quantity that is maybe slightly less defined, but it would be much easier to compute: the function $S_I(r)$ that it is the entropy computed using integrals equations that generalize the hypernetted chain approximation. $S_I(r)$ coincides with the results of the hypernetted chain approximation approximation as soon the bridge diagrams are neglected, but it can be much more complex.

Homework

- The computation of $S_I(r)$ is the more urgent task in order to obtain analytic predictions. While the situations is more or less clear in the HNC, it is not clear if there is a value of the density where bridge diagrams must be considered. Having under control $S_I(r)$ would be very interesting.
- One should extend to the lattice case the analytic tools that are used to predict a glass transition in the hard sphere liquid, in order to see if they predict a phase transition also in $S_L(r)$.
- One should numerically evaluate the quantity $S_L(r)$, at least in low dimensions where numerical computations should be feasible, to see if there are signs of a first order transition by increasing the dimensions.

If we succeed in showing that $S_I(r)$ is well defined, one can put forward the conjecture that

$$S_I(r) = S_L(r) \ .$$

A preliminary test of this conjecture can be done by verifying that the terms that we have neglected in the difference do not pile up to something finite.

In conclusion this paper has posed more problem that those it has solved. The difference and the commonalities of the two problems could be further clarified.

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