Geometric and Probabilistic Aspects of Boson Lattice Models

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ABSTRACT This review describes quantum systems of bosonic particles moving on a lattice. These models are relevant in statistical physics, and have natural ties with probability theory. The general setting is recalled and the main questions about phase transitions are addressed. A lattice model with Lennard–Jones potential is studied as an example of a system where first-order phase transitions occur.

A major interest of bosonic systems is the possibility of displaying a Bose–Einstein condensation. This is discussed in the light of the main existing rigorous result, namely its occurrence in the hard-core boson model. Finally, we consider another approach that involves the lengths of the cycles formed by the particles in the space-time representation; Bose–Einstein condensation should be related to positive probability of infinite cycles.

1 Introduction

Statistical Physics is the study of macroscopic properties of systems with a large number of microsopic particles. Its relevance stems from the law of large numbers, allowing the state of a system to be specified by the values of a few 'macroscopic variables', although the number of microscopic degrees of freedom is enormous. From a probability theory point of view, the Ising model of classical spins is an example of identically distributed, but not independent, random variables; when couplings are small (high temperature, random variables close to independent), magnetization is zero; for large couplings however (strong dependence, or low temperature), the law of large numbers takes a subtler form, with two typical values for the magnetization. This behavior is a manifestation of a phase transition. Connections between statistical physics and probability theory, such as the relation between the physical entropy and the rate function of large deviations, are discussed in detail by Pfister in his excellent lectures [29].

While the original motivation for the Ising model resides in quantum mechanics, it is considered as a classical model, because energy and observables

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are functions on the space of configurations — in quantum systems, these are operators on the vector space spanned by the configurations. There are several reasons for devoting some attention to quantum systems:

- They are closer to the physical reality, and usually of more interest to physicists than classical ones.
- They have richer properties; new types of phases such as superfluidity or superconductivity may show up that are intrinsically quantum phenomena.
- They pose a number of mathematically interesting questions.

There are three classes of quantum lattice systems. The first class consists of spin systems, such as the quantum Heisenberg model, where each site of the lattice hosts a spin that interacts with nearest neighbors. In the second class are fermionic systems, an example of which is the Hubbard model, where the kinetic energy of the quantum particles is provided by a discrete Laplacian ('hopping matrix'), while the potential energy is given by an operator that is a function of the position operators; particles are indistinguishable, so that a permutation of the particles results in the same quantum state, up to a sign for odd permutations. The last class consists in bosonic systems that describe particles hopping on a lattice and interacting among themselves, but a permutation does not alter their wavefunction. There are also other models that have spins and particles, particles with spins, or both kinds of particles.

This review focuses on bosonic systems. They have a great advantage over fermionic ones, namely that the statistical operator $\mathrm{e}^{-\beta H}$ has positive entries in the basis of 'classical configurations'. Hence natural links with probability theory. Bosonic systems also have extremely interesting behavior with various phase transitions, including the Bose–Einstein condensation (hereafter denoted BEC), that should be one of the mechanisms leading to superfluidity and superconductivity. Section 2 introduces the general formalism and defines equilibrium states. This leads to the notion of phase transitions and of symmetry breaking. These ideas are then illustrated in a simple boson model with Lennard–Jones potential; its low temperature phase diagram is analyzed and shown to display various phase transitions (Section 3). This can be proven by showing the equivalence of this model with a 'contour model' that fits the framework of the Pirogov–Sinai theory (Section 4). These techniques, however useful, do not allow discussion of the occurrence of BEC. We briefly review the main questions in Section 5, and state the best result so far — the occurrence of 'off-diagonal long-range order' in the hard-core boson lattice model [12, 20], see Theorem 5.1. We conclude by discussing an approach to the BEC that is both geometric and probabilistic, and that involves the 'cycles' formed by bosonic trajectories in the Feynman–Kac representation. A critical temperature is expected below which the probability of observing an infinite cycle becomes positive, and this transition should be related to BEC. These ideas are described in Section 6.

2 Mathematical Structure

2.1 Microscopic description

The physical picture is that of a group of bosons on a lattice, with the kinetic energy described by a discrete Laplacian, and interacting with a two-body potential.

Let $\Lambda \subset \mathbb{Z}^d$ be a finite domain. The space $\mathbb{C}^\Lambda$ of 'wave functions' on Λ is a Hilbert space, and a normalized vector describes the state of a quantum particle. For $\Psi \in \otimes_{n=1}^N \mathbb{C}^\Lambda$ we define the symmetrization operator S_N,

$$S_N \Psi(x_1, \ldots, x_N) = \frac{1}{N!} \sum_\pi \Psi(x_{\pi(1)}, \ldots, x_{\pi(N)}),$$

where the sum is over all permutations of N elements. Then $S_N(\otimes_{n=1}^N \mathbb{C}^\Lambda)$ is the Hilbert space for N bosonic particles, and the Fock space that describes a variable number of particles is $\mathcal{F}_\Lambda = \oplus_{N=0}^\infty S_N(\otimes^N \mathbb{C}^\Lambda)$. There is a natural inner product on this space that makes it into a Hilbert space.

This formalism is the natural one from a physical point of view, but it is more practical to consider another Hilbert space that is isomorphic to the Fock space above. Thus we start again, this time in the appropriate setting. Standard references are Israel [19] and Simon [31].

We consider a Hilbert space $\mathcal{H}_0$; either $\mathcal{H}_0 \simeq \mathbb{C}^\infty$ (more precisely $\mathcal{H}_0 \simeq \ell^2(\mathbb{C})$), or $\mathcal{H}_0 \simeq \mathbb{C}^N$ for systems with a 'hard-core condition', i.e., a prescription that sets a maximal number N of bosons at a given site. Then we define local Hilbert spaces $\{\mathcal{H}_x\}_{x \in \mathbb{Z}^d}$ where each $\mathcal{H}_x$ is isomorphic to $\mathcal{H}_0$, and for $\Lambda \subset \mathbb{Z}^d$ we set $\mathcal{H}_\Lambda = \otimes_{x \in \Lambda} \mathcal{H}_x$.

A natural basis for $\mathcal{H}_0$ is $\{|n_0\rangle\}_{n_0 \in \mathbb{N}}$; for $\mathcal{H}_\Lambda$, an element of this basis is

$$|n\rangle = \otimes_{x \in \Lambda} |n_x\rangle, \tag{2.1}$$

where $n \in \mathbb{N}^\Lambda$. This represents a state where the site x has n_x bosons. The main operators are the *creation operator* of a boson at site x, noted $c_x^\dagger$, its adjoint the *annihilation operator* c_x, and the *operator number of particles* at x, $\hat{n}_x = c_x^\dagger c_x$. Their actions on members of the above basis are

$$\begin{aligned} c_x^\dagger |n\rangle &= \sqrt{n_x + 1}\, |n + \delta_x\rangle, \\ c_x |n\rangle &= \sqrt{n_x}\, |n - \delta_x\rangle, \\ \hat{n}_x |n\rangle &= n_x |n\rangle. \end{aligned} \tag{2.2}$$

Here, we denoted $|n+\delta_x\rangle$ the vector that is equal to $\otimes_{y \in \Lambda} |n_y + \delta_{xy}\rangle$. Considering a system with hard-core bosons, we demand that $c_x^\dagger |n\rangle = 0$ if $n_x = N$. Notice that the operators $\hat{n}_x$ are diagonal in this basis. Without hard-cores, creation and annihilation operators satisfy the commutation relations

$$[c_x, c_y^\dagger] = \delta_{xy}. \tag{2.3}$$

With a hard-core, the relation is

$$[c_x, c_y^\dagger] = \delta_{xy} \Big\{ 1 - (N+1) \sum_{n : n_x = N} |n\rangle\langle n| \Big\}. \tag{2.4}$$

In order to avoid extra technicalities associated with unbounded operators, we restrict our interest to models with a hard-core condition.

The energy of the particles is given by an 'interaction', that is, a collection of operators $H = (H_A)_{A \subset \mathbb{Z}^d}$ with $H_A : \mathcal{H}_A \to \mathcal{H}_A$. We commit an abuse of notation and still denote H_A the operator $H_A \otimes \mathbb{1}_{\Lambda \setminus A}$. We define operations $(H + H')_A = H_A + H'_A$ and $(\lambda H)_A = \lambda H_A$, and introduce the norm

$$\|H\|_r = \sup_x \sum_{A \ni x} \|H_A\| \, \mathrm{e}^{r\|A\|} \tag{2.5}$$

for some positive number r, where $\|A\|$ is the cardinality of the smallest connected set that contains A. An interaction is periodic iff there exists a finite integer ℓ such that $H_{\tau_x A} = H_A$ for all $x \in \ell\mathbb{Z}^d$. Here, τ_x is the translation operator. We denote by $\mathcal{B}$ the smallest Banach space that contains all *periodic* interactions with finite norm (2.5).

2.2 Free energy and equilibrium states

The *free energy*[1] for a periodic interaction H and at inverse temperature β is

$$f(H) = -\frac{1}{\beta} \lim_{m \to \infty} \frac{1}{|\Lambda_m|} \log \mathrm{Tr} \, \mathrm{e}^{-\beta \sum_{A \subset \Lambda_m} H_A}, \tag{2.6}$$

where Λ_m is a d-dimensional box of size m centered at the origin. The free energy is a concave function of the interactions. Since it is continuous, the definition (2.6) extends to non-periodic interactions in $\mathcal{B}$.

An *equilibrium state* ρ_H for the interaction H is a linear functional on the space of interactions, that is tangent to the free energy at H, i.e., for all $K \in \mathcal{B}$,

$$\rho_H(K) + f(H) \geqslant f(H + K). \tag{2.7}$$

To motivate this definition, let us consider the free energy at finite volume $f_\Lambda(H)$, given by (2.6) without taking the limit. The corresponding finite volume state would be

$$\rho_H^\Lambda(K) = \frac{\mathrm{d}}{\mathrm{d}\lambda} f_\Lambda(H + \lambda K)\Big|_{\lambda=0} = \frac{\mathrm{Tr} \, (\frac{1}{|\Lambda|} \sum_{A \subset \Lambda} K_A) \, \mathrm{e}^{-\beta \sum_{A \subset \Lambda} H_A}}{\mathrm{Tr} \, \mathrm{e}^{-\beta \sum_{A \subset \Lambda} H_A}}.$$

[1] Some authors prefer to define the *pressure* instead, that is equal to $-\beta$ times the free energy. In thermodynamics, the pressure is the potential depending on temperature, volume, and chemical potential. It would be physically more appropriate for the discussion of boson models below. The free energy is however more convenient for low temperature studies, since $\lim_{\beta \to \infty} f(H)$ exists in typical situations.

The definition (2.7) is therefore more general, and allows us to define states directly with the free energy in the limit of infinite volumes. The set of tangent functionals at a given H is a simplex; extremal points are the 'pure states'. Existence of more than one tangent functional implies a *first-order phase transition*.

A popular definition of equilibrium states in quantum lattice systems involves 'KMS states'. Periodic KMS states are actually equivalent to tangent functionals, see e.g., [19, 31].

One could restrict our interest to operators that are diagonal with respect to the basis (2.1) above. In this case, one would consider the configuration space $\mathbb{N}^\Lambda$ and the interactions would be collections of functions on this space. As a result we have a classical system, whose free energy is still given by (2.6). States can also be defined as tangent functionals to the free energy.

Hamiltonians (or interactions, in our case) may possess *symmetries*: for instance, a translation by a vector of the lattice often does not affect the energy, nor does a rotation or a reflection. In quantum statistical physics, one says that $U : \mathcal{B} \to \mathcal{B}$, $H \mapsto H' = U(H)$ is a symmetry if for all m there exists a unitary operator U_m in $\mathcal{H}_{\Lambda_m}$ such that

$$U_m \sum_{A \subset \Lambda_m} H_A \, U_m^{-1} = \sum_{A \subset \Lambda_m} H'_A. \tag{2.8}$$

Clearly, one has $f(H') = f(H)$.

Let us illustrate this notion in two examples that will be relevant in the sequel. The first one is the translation by one site in the direction 1; it is defined by $H'_A = H_{A-e_1}$, where $A - e_1 = \{x : (x(1)+1, x(2), \ldots, x(d)) \in A\}$. Let us assume that the boxes Λ_m are rectangles with periodic boundary conditions, and $1 \leqslant x(1) \leqslant L$. Then one can choose U_m to be $U_m \, |n_{\Lambda_m}\rangle = |n'_{\Lambda_m}\rangle$, where $n'_x = n_{(x(1)-1, x(2), \ldots, x(d))}$ if $x(1) \neq 1$, $n'_x = n_{(L, x(2), \ldots, x(d))}$ if $x(1) = 1$.

The second example is relevant for the Bose–Einstein condensation and is called a 'global gauge symmetry'; U_m takes the form $U_m = \mathrm{e}^{\mathrm{i}\alpha \sum_{x \in \Lambda_m} \hat{n}_x}$, $\alpha \in [0, 2\pi)$. Hamiltonians describing real particles always conserve the total number of particles, and hence possess the global gauge symmetry. It can be broken however, yielding states where the fluctuations of the number of particles in a domain Λ are more than $\sqrt{|\Lambda|}$.[2] We discuss this in Section 5.

[2]Large deviations of the number of particles in a finite domain are studied in [24] in the ideal Bose gas, outside the condensation regime. They are indirectly affected by BEC, if the deviated phase is a condensate.

3 Example: Hopping Particles with Two-body Interactions

In this section we introduce a simple lattice model and study it by means of geometric methods. One obtains that the free energy displays angles corresponding to first-order phase transitions, see Fig. 2 below. Let us mention that the existence of a first-order phase transition in a quantum system *in the continuum* has been recently established for the (quantum) Widom–Rowlinson model [6, 18].

3.1 The model

The particles have kinetic and potential energy, so that the Hamiltonian is

$$H = T + V. \tag{3.1}$$

The kinetic energy T of particles on a lattice is described by a discrete Laplacian that can be written using the creation and annihilation operators in the following way: $T = (T_A)$, with

$$T_A = \begin{cases} -t(c_x^\dagger c_y + c_y^\dagger c_x) & \text{if } A = \{x, y\} \text{ with } |x - y| = 1 \\ 0 & \text{otherwise.} \end{cases} \tag{3.2}$$

We consider here two-body interactions given by a function $U(\cdot)$ that depends on the Euclidean distance between two particles.

$$V_A = \begin{cases} U(|x - y|)\, \hat{n}_x \hat{n}_y & \text{if } A = \{x, y\} \text{ and } x \neq y \\ \frac{1}{2} U(0)\, \hat{n}_x(\hat{n}_x - 1) & \text{if } A = \{x\} \\ 0 & \text{otherwise.} \end{cases} \tag{3.3}$$

The on-site operator $\frac{1}{2}\hat{n}_x(\hat{n}_x - 1)$ is the number of pairs of particles at site x, and the energy is naturally proportional to it. The model with only on-site interactions was introduced in [14] and is usually called the Bose–Hubbard model.

In order for the Hamiltonian $H = T + V$ to have finite norm (2.5), the interaction U must have exponential decay for large distances. The density of the system is controlled by a term involving a chemical potential, $-\mu N$, where N is the 'interaction' that corresponds to the number of particles:

$$N_A = \begin{cases} \hat{n}_x & \text{if } A = \{x\} \\ 0 & \text{if } |A| \geqslant 2. \end{cases} \tag{3.4}$$

Let us now discuss in more detail the case of a Lennard–Jones type of potential; the graph of the corresponding U is depicted in Fig. 1. We suppose that $U(0) = +\infty$, corresponding to a hard-core condition that prevents multiple

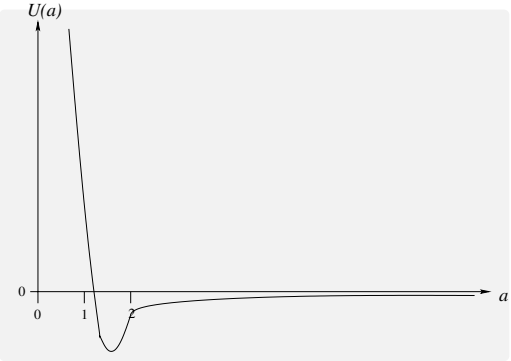

Figure 1. The graph of a Lennard–Jones type of potential.

occupancy of the sites. We will also suppose that

$$u_r = \sum_{|y| \geqslant 2} |U(|y|)|\, \mathrm{e}^{r|y|} \tag{3.5}$$

is small, which amounts to saying that the tail of the potential will not play an important role; the only important values of the potential are $U(1)$ and $U(\sqrt{2})$. The results below are valid for $u_r \leqslant u_0$, the values of u_0 and r depending on $U(1)$ and $U(\sqrt{2})$.

We start with an analysis of the ground states of the 'classical model' with configuration space $\{0,1\}^\Lambda$ and a Hamiltonian given as a sum over squares S of four nearest-neighbor sites:

$$H_\Lambda^{\mathrm{cl}}(n) = \sum_{S \subset \Lambda} \Big[\frac{U(1)}{2(d-1)} \sum_{\substack{\{x,y\} \subset S \\ |x-y|=1}} n_x n_y + U(\sqrt{2}) \sum_{\substack{\{x,y\} \subset S \\ |x-y|=\sqrt{2}}} n_x n_y \Big] - \frac{1}{4} \sum_{x \in S} \big[\mu\, n_x + h\, (-1)^x n_x \big]. \tag{3.6}$$

We added a staggered interaction $-h(-1)^x n_x$, with $(-1)^x \equiv (-1)^{\|x\|_1}$. This interaction has no physical relevance, but is mathematically useful to uncover the occurrence of phases of the chessboard type that breaks the symmetry of translation invariance. One is of course interested in what happens when $h = 0$.

The Hamiltonian above was written as a sum over squares S because it simplifies the analysis of its ground states. It turns out that four configurations are important. The first one is the configuration without particles, where each square is in the configuration $\left(\begin{smallmatrix} 0 & 0 \\ 0 & 0 \end{smallmatrix}\right)$; the second configuration is a chessboard one that is represented by $\left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$; third we have the other chessboard configuration, $\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$; and finally we have a configuration with one particle per site, $\left(\begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix}\right)$. It is

an easy task to compute their respective energy densities; we find

$$\begin{aligned} e^{\mu,h}\left(\begin{smallmatrix}0&0\\0&0\end{smallmatrix}\right) &= 0 \\ e^{\mu,h}\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right) &= U(\sqrt{2}) - \tfrac{\mu}{2} - \tfrac{h}{2} \\ e^{\mu,h}\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right) &= U(\sqrt{2}) - \tfrac{\mu}{2} + \tfrac{h}{2} \\ e^{\mu,h}\left(\begin{smallmatrix}1&1\\1&1\end{smallmatrix}\right) &= 2U(1) + 2U(\sqrt{2}) - \mu. \end{aligned} \tag{3.7}$$

We make the further assumptions on the potential that $U(1) > 0$, ensuring a chessboard phase to be present, and $U(\sqrt{2}) < 0$, so that no phases with quarter density show up — they are more difficult to study, since the classical model has an infinite number of ground states. In many cases one expects that this degeneracy will be lifted as a result of 'quantum fluctuations', that is, the effect of a small kinetic energy T. A general theory of such effects combined with the Pirogov–Sinai theory can be found in [10, 23]. Notice that $U(1) > U(\sqrt{2})$, meaning that at low temperature, the chessboard phase overcomes the phase with alternate rows or columns of 1's and 0's. Energies (3.7) provide the zero-temperature phase diagram and allow guesses for the low temperature situation.

3.2 The phase diagram

The situation at high temperature (β small) is that of bosons with weak interactions and no phase transitions may occur. The natural condition for high temperature is that $\beta\|H\|_r$ is small; one can however prove slightly more by *not* requesting that $U(0)$ be small. So we define (compare with (2.5))

$$\|H\|_r^* = \sup_x \sum_{\substack{A \ni x \\ |A| \geqslant 2}} \|H_A\| \, \mathrm{e}^{r\|A\|} \,. \tag{3.8}$$

Theorem 3.1. *There exists $r < \infty$ such that if $\beta\|H\|_r^* < 1$, there is a unique tangent functional at H, and for any $K \in \mathcal{B}$ the free energy $f(H + \eta K)$ is real analytic in η in a neighborhood of 0.*

This theorem is proven in Section 4.4 using high temperature expansions, following [36]. We shall see below that there may be more than one tangent functional at low temperature, corresponding to equilibrium states that are not translation invariant. This implies that a transition with symmetry breaking takes place when the temperature decreases. Presumably it is second order (the second derivative of the free energy with respect to β has a discontinuity), as in the Ising model, but there are no rigorous results to support this.

The limit $\beta \to \infty$ is easily analyzed and is depicted in Fig. 2.

The graph of the function $e^{\mu,h}$ is a kind of roof with four flat parts. There are angles between each flat part, so that first derivatives have discontinuities there. The two questions that should be asked are:

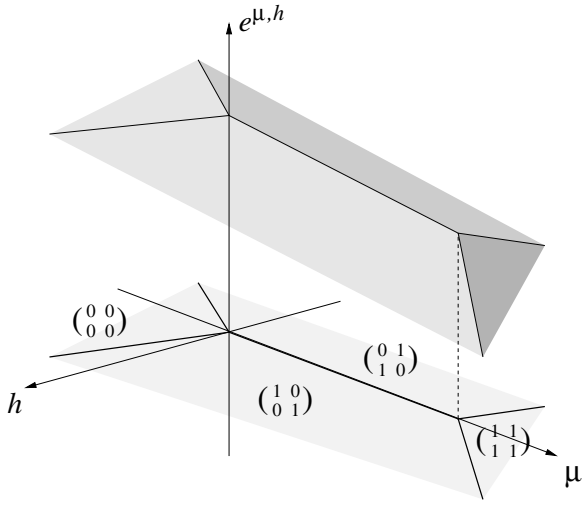

Figure 2. The free energy in the limit $\beta \to \infty$. The phase diagram is divided in four domains, corresponding to the empty, chessboards, and full configurations. For large β and small t, the flat parts bend but the angles remain.

- Does this picture survive when adding the tail of the potential, and the kinetic energy (hopping matrix)?
- Does this picture survive at non-zero temperatures?

The answer to both questions is yes and is provided by the *quantum Pirogov–Sinai theory*. It can be viewed as a considerable extension of the Peierls argument for the Ising model. It was proposed by Pirogov and Sinai for classical lattice models [30, 32], and extended to quantum models in [3, 9, 10, 23, 15]. These ideas are discussed for this model in the next section. One is then led to the phase diagram of Fig. 3.

Multiple phases and occurrences of first order phase transitions are proven when β is large and t small, i.e., at low temperature and close to the classical limit of vanishing hoppings. It is expected that BEC and superfluidity are present in dimension $d \geqslant 3$, when the temperature is low and with sufficient hoppings [14]. Actually, the situation $U(0) = \infty$ and $U(a) = 0$ for $a \geqslant 1$ corresponds to the hard-core boson model, when BEC is proven at low temperature [12, 20]; see Section 5.

The proof of existence of phase transitions was obtained in [3, 9]; it was realized in [15] that tangent functionals naturally fit in the context of the Pirogov–Sinai theory.

The zero-temperature energy takes the form (see Fig. 2)

$$e^{\mu,h} = \min_{\left(\begin{smallmatrix}\cdot&\cdot\\\cdot&\cdot\end{smallmatrix}\right)} e^{\mu,h}\left(\begin{smallmatrix}\cdot&\cdot\\\cdot&\cdot\end{smallmatrix}\right) \tag{3.9}$$

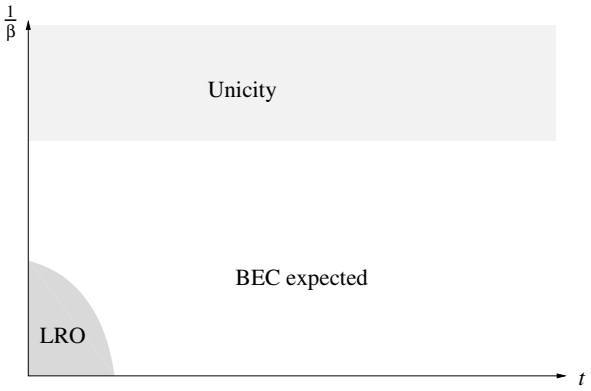

Figure 3. The phase diagram $(t, \frac{1}{\beta})$ of the boson model with Lennard–Jones potential. There is a unique state (tangent functional) at high temperature, while a domain with two extremal states, and hence long-range order (LRO), is present for low temperature and small hopping (darker zone). Most of the phase diagram is not rigorously understood yet.

where the minimum is taken over the four configurations $\left(\begin{smallmatrix}0&0\\0&0\end{smallmatrix}\right)$, $\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right)$, $\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)$, and $\left(\begin{smallmatrix}1&1\\1&1\end{smallmatrix}\right)$. There are angles at the intersections between different energies. It is not clear whether they are present at positive temperature however — an example where angles disappear is the one-dimensional Ising model. The main result of the Pirogov–Sinai theory, in this model, is the claim that there exist four C^1 functions that are close to the energies (3.7), and that play the same role: the free energy is given by the minimum of these four functions, and hence has angles at their intersections.

Theorem 3.2 (Free energy at low temperature). *Assume $d \geqslant 2$. Let $U(0) \to \infty$, $U(1) > 0$ and $U(\sqrt{2}) < 0$. There exist $\beta_0, r < \infty$ such that if $\beta \geqslant \beta_0$ and $t + u_r \leqslant 1$, there are real functions $f^{\mu,h}_{\left(\begin{smallmatrix}0&0\\0&0\end{smallmatrix}\right)}$, $f^{\mu,h}_{\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right)}$, $f^{\mu,h}_{\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)}$, $f^{\mu,h}_{\left(\begin{smallmatrix}1&1\\1&1\end{smallmatrix}\right)}$ such that*

- $$\lim_{\substack{\beta\to\infty\\ t,u_r\to 0}} f^{\mu,h}_{\left(\begin{smallmatrix}\cdot&\cdot\\\cdot&\cdot\end{smallmatrix}\right)} = e^{\mu,h}\left(\begin{smallmatrix}\cdot&\cdot\\\cdot&\cdot\end{smallmatrix}\right) \qquad \text{and} \qquad \lim_{\substack{\beta\to\infty\\ t,u_r\to 0}} \frac{\partial}{\partial\mu,h} f^{\mu,h}_{\left(\begin{smallmatrix}\cdot&\cdot\\\cdot&\cdot\end{smallmatrix}\right)} = \frac{\partial}{\partial\mu,h} e^{\mu,h}\left(\begin{smallmatrix}\cdot&\cdot\\\cdot&\cdot\end{smallmatrix}\right)$$

  uniformly in μ, h. Limits are taken in any order. The limit $u_r \to 0$ means that $U(a) \to 0$ for all $a \geqslant 2$.

- *The free energy* (2.6) *is given by*

$$f^{\mu,h} = \min_{\left(\begin{smallmatrix}\cdot&\cdot\\\cdot&\cdot\end{smallmatrix}\right)} f^{\mu,h}_{\left(\begin{smallmatrix}\cdot&\cdot\\\cdot&\cdot\end{smallmatrix}\right)}.$$

- *The functions are C^1 in μ, h with uniformly bounded derivatives. Furthermore, $f^{\mu,h}_{\left(\begin{smallmatrix}\cdot & \cdot\\ \cdot & \cdot\end{smallmatrix}\right)}$ is real analytic in μ, h when $f^{\mu,h}_{\left(\begin{smallmatrix}\cdot & \cdot\\ \cdot & \cdot\end{smallmatrix}\right)}$ is the unique minimum.*

The phase diagram is therefore governed by these four functions; clearly, it is symmetric under the transformation $h \to -h$. Let μ_1 be the coexistence point of $\left(\begin{smallmatrix}0 & 0\\ 0 & 0\end{smallmatrix}\right)$ and the chessboards, i.e.,

$$f^{\mu_1,0}_{\left(\begin{smallmatrix}0 & 0\\ 0 & 0\end{smallmatrix}\right)} = f^{\mu_1,0}_{\left(\begin{smallmatrix}0 & 1\\ 1 & 0\end{smallmatrix}\right)}, \tag{3.10}$$

and μ_2 be the coexistence between the chessboard and $\left(\begin{smallmatrix}1 & 1\\ 1 & 1\end{smallmatrix}\right)$. There are exactly two extremal tangent functionals for $\mu_1 < \mu < \mu_2$ and $h = 0$. Exactly three for $\mu = \mu_1$ and $h = 0$, as well as for $\mu = \mu_2$ and $h = 0$. There is a unique tangent functional everywhere else.

Among the consequences are various first-order phase transitions. For instance,

$$\frac{\partial}{\partial h} f^{\mu,h}\Big|_{h=0-} \neq \frac{\partial}{\partial h} f^{\mu,h}\Big|_{h=0+} \tag{3.11}$$

for $\mu_1 < \mu < \mu_2$; also, if $h = 0$,

$$\frac{\partial}{\partial \mu} f^{\mu,0}\Big|_{\mu=\mu_1-} \neq \frac{\partial}{\partial \mu} f^{\mu,0}\Big|_{\mu=\mu_1+}, \tag{3.12}$$

and similarly at μ_2.

Construction of the functions ('metastable free energies' in the Pirogov–Sinai terminology) is done in two steps. First, using a space-time representation of the model, one defines an equivalent *contour model*. This step is explained in the next section; it gives the opportunity to make the link with a stochastic process of classical particles jumping on the lattice. The second step is to get an expression for the metastable free energies starting from a contour model, and this is achieved using the standard Pirogov-Sinai theory [30, 32]. This is only outlined here. Ideas are described e.g., in [21]. It was understood in [15] that tangent functionals to the free energy can be described by the Pirogov–Sinai theory. Further references can be found in [21, 15].

3.3 Incompressibility

The space-time contour representation actually allows us to obtain more. The total number of particles is conserved, and as a consequence the ground state of the quantum model has the same density as for the model without the hopping terms, and hence the compressibility is zero. These observations were made in [4], leading to Theorem 3.3.

If ρ denotes a state, then the corresponding density is $\rho(N)$, where N is the interaction that corresponds to the number of particles, see (3.4). $\rho(N)$ depends

on the chemical potential μ. One defines the *compressibility* κ_{T},

$$\kappa_{\mathrm{T}} = \frac{\partial}{\partial \mu} \rho(N) \tag{3.13}$$

where the derivative is taken at constant temperature $1/\beta$. The theorem below claims incompressibility of the ground state, and also that the low temperature states are close to being incompressible. The state ρ_0 is the one obtained by taking the limits $t \to 0$, $u_r \to 0$, and $\beta \to \infty$. The theorem holds in any dimension.

Theorem 3.3. *Let $U(0) \to \infty$, $U(1) > 0$ and $U(\sqrt{2}) < 0$. There exist $\beta_0, r < \infty$ such that if $\beta \geqslant \beta_0$ and $t + u_r \leqslant 1$, one has*

$$\begin{aligned} &\big|\rho(N) - \rho_0(N)\big| \leqslant C\, \mathrm{e}^{-\beta r'}\,; \\ &|\kappa_{\mathrm{T}}| \leqslant C\, \mathrm{e}^{-\beta r'} \end{aligned}$$

for some constants $C < \infty$, $r' > 0$ (that depend on d, β_0, and r only).

4 The Space-time Representation and the Equivalent Contour Model

4.1 Equivalence with a stochastic system

We start with the finite volume expression for the free energy; for $\Lambda \subset \mathbb{Z}^d$,

$$f_\Lambda = -\frac{1}{\beta|\Lambda|} \log \mathrm{Tr}\ \mathrm{e}^{-\beta \sum_{A \subset \Lambda} H_A}\,, \tag{4.1}$$

where $H = T + V - \mu N$ (we set $h = 0$ for simplification). Notice that the last two interactions are diagonal with respect to the basis (2.1).

One can give various probabilistic interpretations for (4.1), see e.g., [35]. A natural one is a continuous-time Markov chain where the collection of random variables $\{n(t)\}_{t \geqslant 0}$ takes values in $\{0, \dots, N\}^\Lambda$. Let us introduce the set of 'neighbors' of a configuration n:

$$\mathcal{N}(n) = \{n' : \exists x, y \text{ with } |x - y| = 1 \text{ and } n'_z = n_z - \delta_{zx} + \delta_{zy} \text{ for all } z \in \Lambda\}. \tag{4.2}$$

The generator of this random process is

$$G_{nn'} = \begin{cases} 1 & \text{if } n' \in \mathcal{N}(n) \\ -|\mathcal{N}(n)| & \text{if } n' = n \\ 0 & \text{otherwise.} \end{cases} \tag{4.3}$$

The *partition function* $Z_\Lambda = \operatorname{Tr} \mathrm{e}^{-\beta \sum_{A \subset \Lambda} H_A}$ is the expectation

$$Z_\Lambda = \mathbb{E}_{[0,\beta]}\Bigg(\chi[n(0) = n(\beta)] \exp\Big\{ - \int_0^\beta \mathrm{d}\tau \Big[\sum_{x,y \in \Lambda} U(|x-y|) n_x(\tau) n_y(\tau) - \mu \sum_{x \in \Lambda} n_x(\tau) \Big] \Big\} \Bigg). \quad (4.4)$$

Here, $\chi[\cdot]$ is the characteristic function, that is 0 or 1 whenever $\cdot$ is false or true, respectively.

Another representation that is more appealing for the physical intuition involves continuous-time simple random walks. It was outlined in [7] and used to obtain a bound on the free energy of the Heisenberg model [8, 35]. Let $\{x_j(t)\}_{t \geqslant 0}$, $1 \leqslant j \leqslant N$, be random walks, each with the same generator

$$L_{xy} = \begin{cases} 1 & \text{if } |x-y| = 1 \\ -2d & \text{if } x = y \\ 0 & \text{otherwise.} \end{cases} \quad (4.5)$$

Then the partition function takes the form

$$Z_\Lambda = \sum_{N \geqslant 0}^\infty \frac{\mathrm{e}^{\beta \mu N}}{N!} \sum_{x_1, \ldots, x_N \in \Lambda} \sum_{\pi \in S_N} \mathbb{E}\Bigg(\chi\big[x_i(\beta) = x_{\pi(i)}, 1 \leqslant i \leqslant N\big] \exp\Big\{ - \int_0^\beta \mathrm{d}\tau \sum_{i<j} U(|x_i(\tau) - x_j(\tau)|) \Big\} \Big| \, x_i(0) = x_i, 1 \leqslant i \leqslant N \Bigg). \quad (4.6)$$

Here particles have to start and end in Λ, but they are meanwhile free to move outside. One could impose more stringent boundary conditions, by defining a generator L^Λ_{xy} that does not allow particles to leave or enter Λ, or by adding an infinite potential outside of Λ. The free energies corresponding to these various partition functions have the same thermodynamic limit, however.

Notice the sum over permutations in (4.6); this suggests considering probability on sets of permutations, for instance the probability that the permutation has infinite cycles. We discuss this in Section 6, where (4.6) is heuristically important.

Let us mention another example of close ties between quantum systems and probability theory: Aizenman and Nachtergaele showed the equivalence of a quantum spin chain with a stochastic process, which is then equivalent to a two-dimensional Potts model [1]. Using results established for the latter, the authors can draw new conclusions on the former.

4.2 Equivalence with a contour model

A way to derive these stochastic representations is by using the Duhamel formula: if $\boldsymbol{A}$ and $\boldsymbol{B}$ are two matrices, then

$$\begin{aligned} \mathrm{e}^{\boldsymbol{A}+\boldsymbol{B}} &= \mathrm{e}^{\boldsymbol{A}} + \int_0^1 \mathrm{d}\tau\, \mathrm{e}^{\tau\boldsymbol{A}}\, \boldsymbol{B}\, \mathrm{e}^{(1-\tau)(\boldsymbol{A}+\boldsymbol{B})} \\ &= \mathrm{e}^{\boldsymbol{A}} + \sum_{m\geqslant 1} \int_{0<\tau_1<\cdots<\tau_m<1} \mathrm{d}\tau_1 \ldots \mathrm{d}\tau_m\, \mathrm{e}^{\tau_1\boldsymbol{A}}\, \boldsymbol{B}\, \mathrm{e}^{(\tau_2-\tau_1)\boldsymbol{A}}\, \boldsymbol{B} \ldots \boldsymbol{B}\, \mathrm{e}^{(1-\tau_m)\boldsymbol{A}}. \end{aligned} \tag{4.7}$$

Let us set $\boldsymbol{A} = \sum_{A\subset\Lambda}(V_A - \mu N_A - hP_A)$, with P denoting the staggered interaction, and $\boldsymbol{B} = \sum_{A\subset\Lambda} T_A$. We take the trace, introduce $\mathbb{1} = \sum_n |n\rangle\langle n|$ on the right of each operator $\boldsymbol{B}$, and we get the following expression:

$$\begin{aligned} Z_\Lambda = \sum_{m\geqslant 0} (-1)^m \sum_{A_1,\ldots,A_m} \sum_{n_1,\ldots,n_m} \int_{0<\tau_1<\cdots<\tau_m<\beta} \mathrm{d}\tau_1 \ldots \mathrm{d}\tau_m \\ \mathrm{e}^{-\tau_1 H_\Lambda(n_1)} \langle n_1|\, T_{A_1}\, |n_2\rangle\, \mathrm{e}^{-(\tau_2-\tau_1)H_\Lambda(n_2)} \langle n_2|\, T_{A_2}\, |n_3\rangle \ldots \\ \ldots \langle n_m|\, T_{A_m}\, |n_1\rangle\, \mathrm{e}^{-(\beta-\tau_m)H_\Lambda(n_1)}, \end{aligned} \tag{4.8}$$

where we introduced $H_\Lambda(n) = \sum_{A\subset\Lambda}\langle n|\, H_A\, |n\rangle$. One recognizes (4.4) and (4.6). Indeed, the sum over $\{A_i\}$ is actually over pairs of nearest neighbors; $\langle n_1|\, T_{\{x,y\}}\, |n_2\rangle$ is zero unless n_2 is a 'neighbor' of n_1, i.e., it is the same as n_1 up to one particle that moved from x to y, or from y to x. $\{\mathrm{e}^{-(\tau_j-\tau_{j-1})H_\Lambda(n_j)}\}$ is finally represented in (4.4) and (4.6) by the exponential.

To each choice of m, $\{A_j\}$, $\{n_j\}$, $\{\tau_j\}$, corresponds a space-time picture illustrated in Fig. 4. We write $\boldsymbol{n}(\tau)$ for the configuration at time τ, that is, $\boldsymbol{n}(\tau) = n_j$ if $\tau_{j-1} \leqslant \tau < \tau_j$.

The goal is to extract some information on the analytic properties of the free energy, that is, the logarithm of the partition function. A technique that was proposed in 1975 for the study of extensions of the Ising model is the Pirogov–Sinai theory [30, 32], which was later extended to quantum systems in [3, 9, 10, 23, 15]. The strategy is to map the quantum system onto a 'contour model'. The latter is a model where the states are not configurations or vectors of a Hilbert space, but sets of mutually disjoint contours; the statistical weight $\mathrm{e}^{-\beta H}$ is replaced by a product of individual weights for each contour.

Let us describe in detail the setting of a contour model.

A *contour* $\mathcal{A}$ is a pair (A,α), where the *support* A is a connected subset of $\mathbb{Z}^d$. In order to define α, let us introduce the closed unit cell $C(x) = [x-\frac{1}{2}, x+\frac{1}{2}]^d \subset \mathbb{R}^d$ centered at x; the *boundary* $B(A)$ of $A \subset \mathbb{Z}^\nu$ is

$$B(A) = \bigcup_{x\in A, y\notin A} \Big(C(x)\cap C(y)\Big). \tag{4.9}$$

The boundary $B(A)$ decomposes into connected components; each connected component b is given a label $\alpha_b \in \{1,\ldots,p\}$, and $\alpha = (\alpha_b)$.

Let $\Lambda \subset \mathbb{Z}^d$ finite, with periodic boundary conditions. A set of contours $\{\mathcal{A}_1, \ldots, \mathcal{A}_k\}$ is *admissible* iff

- $A_i \subset \Lambda$ for all i, and $\mathrm{dist}\,(A_i, A_j) \geqslant 1$ if $i \neq j$.
- Labels α_j are matching in the following sense. Let $W = \Lambda \setminus \cup_{j=1}^{k} A_j$, then each connected component of W must have the same label on its boundaries.

For $j \in \{1, \ldots, p\}$, let W_j be the union of all connected components of W with labels j on their boundaries.

The partition function of a contour model has the form

$$Z_\Lambda = \sum_{\{\mathcal{A}_1, \ldots, \mathcal{A}_k\}} \prod_{j=1}^{k} w(\mathcal{A}_j) \prod_{i=1}^{p} \mathrm{e}^{-\beta e_i |W_i|}\,, \tag{4.10}$$

where the sum is over admissible sets of contours in Λ.

The *weight* $w(\mathcal{A})$ of a contour $\mathcal{A}$ is a complex function of the temperature and of the parameters of the phase diagram (here μ and h) that is real anlaytic in all these parameters. Furthermore, we need that

$$|w(\mathcal{A})| \leqslant \mathrm{e}^{-\beta e_0 |A|}\ \mathrm{e}^{-r|A|} \tag{4.11}$$

for a large enough constant r (depending on d and p). This typically holds when β is large. We also need that partial derivatives of the weights with respect to μ and h satisfy the same bounds.

Many classical lattice models have such a representation. The usual way to define a contour model is to attribute a set of contours to each configuration. One is given a finite set of periodic configurations ('low energy configurations', or 'reference configurations'), and one defines 'excited sites' as those sites whose neighborhood does not agree with any of the reference configurations. The set of excited sites decompose into connected components, that are supports of the contours. Outside the contours the configuration agrees with one of the reference configurations, and the labels indicate with which one.

The labels are important because the weight of a contour typically depends on which configuration lies outside. If we want this weight to depend on the contour only, we need to provide the information contained in the labels.

We are looking for a similar approach here with the space-time representation. On the one hand, we expect the phase diagram to display four phases: a phase with very low density, corresponding to $\left(\begin{smallmatrix} 0 & 0 \\ 0 & 0 \end{smallmatrix}\right)$; two chessboard phases, $\left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ and $\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$; and a phase with density close to 1, $\left(\begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix}\right)$. These are our reference configurations. On the other hand, we suppose here that particles have small hoppings, so that jumps are typically rare in Fig. 4.

In order to get contours that have supports on a lattice, we discretize the continuous direction. Let $\tilde{\beta}$ be such that $\beta = M\tilde{\beta}$ with M an integer. We consider the lattice $\mathbf{\Lambda} = \Lambda \times \{1, \ldots, M\}$. A site $\boldsymbol{x} = (x, s) \in \mathbf{\Lambda}$ is 'in the state

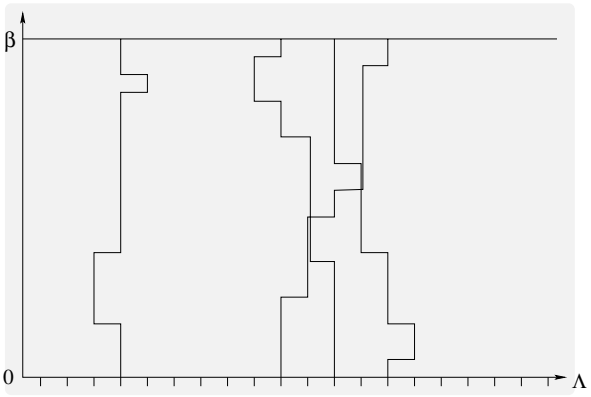

Figure 4. Space-time representation of the partition function as expanded in (4.8). There are four bosonic trajectories in this picture.

$\left(\begin{smallmatrix}0&0\\0&0\end{smallmatrix}\right)$' if for all y with $|y-x| \leqslant 1$, and all $(s-1)\tilde{\beta} < \tau < s\tilde{\beta}$, we have $\boldsymbol{n}_y(\tau) = 0$. We make similar definitions for the other three reference configurations.

Cells that are not in such a state are called *excited*. Connected components of the set of excited cells are the supports of the contours, and labels take values in $\{\left(\begin{smallmatrix}0&0\\0&0\end{smallmatrix}\right), \left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right), \left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right), \left(\begin{smallmatrix}1&1\\1&1\end{smallmatrix}\right)\}$ and contain information on which configuration touches the support. This is illustrated in Fig. 5.

Summing first over contour configurations, then integrating over compatible

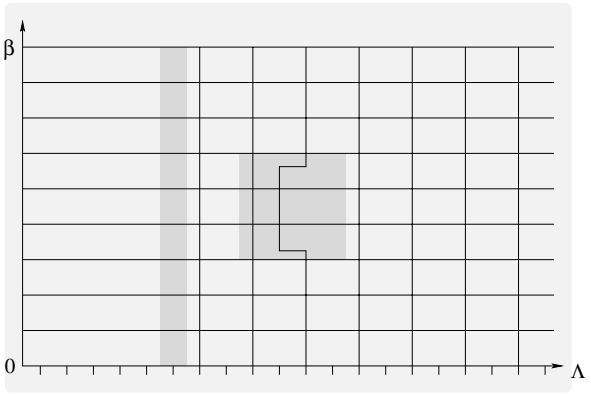

Figure 5. Contours in the space-time representation. The contour on the left separates the empty configuration from a chessboard one, while the one on the right is due to the motion of a particle.

space-time configurations, we can rewrite (4.8) as

$$Z_\Lambda = \sum_{\{\mathcal{A}_1,\dots,\mathcal{A}_k\}} \prod_{i=1}^{k} w(\mathcal{A}_i) \prod_{i=1}^{4} \mathrm{e}^{-\tilde{\beta} e_i |W_i|}\,. \tag{4.12}$$

The expression for the weight $w(\mathcal{A})$ is complicated, but the exponential bound (4.11) is not too hard to obtain. It will require $\tilde{\beta}\Delta$ to be large, and $\tilde{\beta}t$ to be small. Theorem 3.2 is then a result of the Pirogov–Sinai theory.

4.3 Consequences of the contour representation

A few words need to be added in view of Theorem 3.3. The density is

$$\rho = \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{\mathrm{Tr}\left(\frac{1}{|\Lambda|}\sum_{x\in\Lambda} \hat{n}_x\right) \mathrm{e}^{-\beta \sum_{A\subset\Lambda} H_A}}{Z_\Lambda}. \tag{4.13}$$

This expression for the density agrees with the derivative of the free energy with respect to μ, provided it is differentiable. Indeed, we consider the free energy $f(H-\mu N)$ as a function of the chemical potential. It is concave, and if it is differentiable at μ we have

$$\rho = -\frac{\mathrm{d}}{\mathrm{d}\mu} f(H-\mu N) = -\lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{\mathrm{d}}{\mathrm{d}\mu} f_\Lambda(H-\mu N). \tag{4.14}$$

The space-time expansion of (4.13) was studied in [4]. Due to the conservation of the total number of particles, differences between the density of the quantum model (with hoppings) and the classical one (without hoppings) lead to contours that wind around the torus $\Lambda \times [0,\beta]_{\mathrm{per}}$. Hence their length is at least β, and no such contours survive when taking the limit $\beta \to \infty$. As a consequence, the density of the quantum model is locked to the classical one.

This clearly implies that the compressibility vanishes at zero temperature. To obtain the low temperature bounds requires some more work, that also goes through an expansion involving winding contours [4].

4.4 Proof of Theorem 3.1

We conclude this section by proving that there is a unique equilibrium state at high temperature, as stated in Theorem 3.1. It strongly relies on ideas discussed above, with many simplifications. We show the equivalence between the quantum model and a *polymer model* — this is a contour model without labels (i.e., $p = 1$). Once we have obtained this equivalence, the results follow from cluster expansions [22, 11, 5].

We consider the partition function for the interaction $(H + \eta K)$, that we expand using the Duhamel formula (4.7). Let H' be

$$H'_A = \begin{cases} K_{\{x\}} & \text{if } A = \{x\} \\ H_A + K_A & \text{if } |A| \geqslant 2. \end{cases} \tag{4.15}$$

Then

$$\begin{aligned}\mathrm{Tr}\ \mathrm{e}^{-\beta\sum_{A\subset\Lambda}(H_A+\eta K_A)} &= \mathrm{Tr}\ \mathrm{e}^{-\beta\sum_{x\in\Lambda}H_{\{x\}}} \\ &+ \sum_{m\geqslant 1}(-1)^m \sum_{A_1,\dots,A_m} \int_{0<\tau_1<\dots<\tau_m<\beta} \mathrm{d}\tau_1\dots\mathrm{d}\tau_m \\ &\mathrm{Tr}\ \mathrm{e}^{-\tau_1\sum_x H_{\{x\}}} H'_{A_1} \mathrm{e}^{-(\tau_2-\tau_1)\sum_x H_{\{x\}}} H'_{A_2}\dots H'_{A_m} \mathrm{e}^{-(\beta-\tau_m)\sum_x H_{\{x\}}}. \quad (4.16)\end{aligned}$$

Let $F_x^{(0)}$ be defined by

$$\mathrm{e}^{-\beta F_x^{(0)}} = \mathrm{Tr}\ \mathrm{e}^{-\beta H_{\{x\}}}, \quad (4.17)$$

with the trace taken in the single-site Hilbert space $\mathcal{H}_x$. We define polymers as connected components of the set $\cup_{j=1}^m A_j$, and the weight of a polymer A to be

$$\begin{aligned}w(A) = \mathrm{e}^{\beta\sum_{x\in A}F_x^{(0)}} &\sum_{m\geqslant 1}(-1)^m \sum_{\substack{A_1,\dots,A_m \\ \cup_j A_j = A}} \int_{0<\tau_1<\dots<\tau_m<\beta} \mathrm{d}\tau_1\dots\mathrm{d}\tau_m \\ &\mathrm{Tr}\ \mathrm{e}^{-\tau_1\sum_{x\in A}H_{\{x\}}} H'_{A_1} \mathrm{e}^{-(\tau_2-\tau_1)\sum_x H_{\{x\}}} \dots \mathrm{e}^{-(\beta-\tau_m)\sum_{x\in A}H_{\{x\}}}. \quad (4.18)\end{aligned}$$

Then

$$\mathrm{Tr}\ \mathrm{e}^{-\beta\sum_{A\subset\Lambda}H_A} = \mathrm{e}^{-\beta\sum_{x\in\Lambda}F_x^{(0)}} \sum_{\{A_1,\dots,A_k\}} \prod_{j=1}^k w(A_j). \quad (4.19)$$

This is the partition function of a polymer model.

We need a bound on the weight of the polymers. Since the dimension of the Hilbert space $\mathcal{H}_A$ is $(N+1)^{|A|}$, we can estimate the last line of (4.18) by

$$\mathrm{Tr}\ \cdot\ \leqslant (N+1)^{|A|} \prod_{x\in A} \|\,\mathrm{e}^{-\beta H_{\{x\}}}\,\| \prod_{j=1}^m \|H'_{A_j}\|. \quad (4.20)$$

Furthermore,

$$\|\,\mathrm{e}^{-\beta H_{\{x\}}}\,\| \leqslant \mathrm{e}^{-\beta F_x^{(0)}}, \quad (4.21)$$

so we obtain

$$\begin{aligned}|w(A)| &\leqslant (N+1)^{|A|}\,\mathrm{e}^{-r|A|} \sum_{m\geqslant 1} \frac{\beta^m}{m!} \Big(\sum_{A'\subset A} \|H'_{A'}\|\,\mathrm{e}^{r|A'|}\Big)^m \\ &\leqslant \mathrm{e}^{|A|\log(N+1)}\ \mathrm{e}^{-r|A|}\ \mathrm{e}^{\beta|A|\|H'\|_r}. \quad (4.22)\end{aligned}$$

For η small we have

$$\beta\|H'\|_r \leqslant \beta\|H\|_r^* + \beta|\eta|\,\|K\| \leqslant 1, \quad (4.23)$$

so that the weights satisfy the assumptions of the cluster expansions provided $r - \log(N+1) - 1$ is large enough (depending on d only). One then obtains an exact expression for the infinite volume free energy: in the translation invariant case ($F_x = F_y$ and $w(A+x) = w(A)$), the mean free energy is given by

$$f(H + \eta K) = F_0^{(0)} - \frac{1}{\beta} \sum_{(A_1,\dots,A_k)} \varphi^{\mathrm{T}}(A_1, \dots, A_k) \prod_{j=1}^{k} w(A_j), \tag{4.24}$$

with the sum over *clusters*, that is, k-tuples $(A_1, \dots, A_k)$, $k \geqslant 1$, such that their union $\cup_{j=1}^{k} A_j$ is connected. The combinatoric factor $\varphi^{\mathrm{T}}(A_1, \dots, A_k)$ has an expression involving the graph of k vertices with an edge between i and j whenever $A_i \cup A_j$ is connected. The results on cluster expansions include bounds ensuring the convergence of the sum (4.24); see e.g., [22, 11, 5] for detailed results and proofs.

By averaging over a cell whose dimensions are given by the periods of the interactions, one obtains a similar expression in the case of periodicity rather than translation invariance.

It is clear that the weights are analytic as a function of η. Since the free energy $f(H + \eta K)$ is given by a convergent sum of clusters, it is real analytic, and there is a unique tangent functional at H.

5 A Discussion of the Bose–Einstein Condensation

5.1 The origins

The story started in 1924 when Satyendra Nath Bose sent a paper to Albert Einstein, that was previously rejected by *Philosophical Magazine*. Einstein translated it into German and recommended its publication in *Zeitschrift für Physik*; he wrote articles shortly afterwards in *Sitzungsberichte Preussische Akademie der Wissenschaften* (1924–25). The 'Bose–Einstein statistics' for quantum particles (in particular photons) was uncovered, and a curious phase transition was proposed, where the ground state of the one-particle Hamiltonian is macroscopically occupied. This is the *Bose–Einstein condensation* for the *ideal* boson gas (that is, without interactions).

For some time it was not clear whether such a transition was really occurring in nature; but London proposed in 1938 that superfluidity in Helium was a consequence of a Bose–Einstein condensation, an idea that is largely accepted nowadays.

Is there a condensation for interacting systems as well, and what does it mean? These questions were addressed by Feynman [13]; he suggested the idea that the transition corresponds to positive probability for the occurrence of infinite cycles in the space-time representation — this will be discussed in greater detail in the next section. Feynman's conclusion is that weakly interacting systems behave like non-interacting ones, albeit with a larger effective mass, and

still display condensation.

Direct experimental evidence of BEC has been observed only recently [2].

5.2 General ideas

A system of N bosons in the continuum is described by the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \sum_{j=1}^{N} \Delta_j + \sum_{i<j} U(|x_i - x_j|). \tag{5.1}$$

Here, Δ_j is the Laplace operator $\sum_{\alpha=1}^{d} \frac{\partial^2}{\partial x_{j,\alpha}^2}$ and x_j is the position of the j-th particle. The low temperatures should be described by the Bogolubov theory, see e.g., [25, 37] for an introduction and partial justification. The Bogolubov theory relies on the assumption that most of the particles are in the ground state of the Laplace operator (that is, the Hamiltonian for the ideal gas), which is false in presence of interactions. Still, many predictions are correct; in particular, it gives a value for the ground state energy per particle e_0 at low density,

$$e_0 = \frac{2\pi\hbar^2\rho a}{m}\big(1 + o(\rho a^3)\big), \tag{5.2}$$

where ρ is the density and a is the scattering length of the potential U. This formula has been rigorously established by Lieb and Yngvason [27]. This and other results are reviewed in [26].

Further developments led to the concept of *off-diagonal long-range order* due to Penrose and Onsager [28]. Take e.g., the lattice model of Section 3. One considers the following order parameter:

$$\langle c_x^\dagger c_y \rangle = \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{\operatorname{Tr} c_x^\dagger c_y \, \mathrm{e}^{-\beta \sum_{A \subset \Lambda} H_A}}{\operatorname{Tr} \mathrm{e}^{-\beta \sum_{A \subset \Lambda} H_A}} \tag{5.3}$$

where $H = T + V - \mu N$, and the traces are in the Hilbert space $\otimes_{x \in \Lambda} \mathcal{H}_x$. Here, it is natural to set periodic boundary conditions for Λ. The question is:

Does $\lim_{|x-y|\to\infty} \langle c_x^\dagger c_y \rangle$ *differ from 0?*

The equilibrium state at high temperature is unique and clustering, see Theorem 3.1, and hence BEC must be sought at low temperatures.

5.3 The hard-core boson lattice model

There is only one rigorous result establishing the existence of condensation in a reasonable model of interacting bosons. This is a lattice model where bosons interact with hard-core repulsion, i.e., the Hamiltonian (3.1) with $U(0) \to \infty$ and $U(a) \to 0$ if $a \geqslant 1$. The theorem below is due to Dyson, Lieb and Simon [12], and Kennedy, Lieb and Shastry [20]. It is stated for three or more dimensions and at low temperature, but it also holds for the ground state of the 2-dimensional model [20].

Theorem 5.1. *Take $d \geqslant 3$, $H = T + V$ with $U(0) \to \infty$, $U(a) \to 0$ for $a > 0$. Then there is $\beta_0 < \infty$ such that for $\beta > \beta_0$,*

$$\lim_{|x-y|\to\infty} \langle c_x^\dagger c_y \rangle \neq 0.$$

This theorem implies the existence of a phase transition in the sense that the state $\langle\cdot\rangle$ is not clustering. It is established using 'reflection positivity', introduced in [16] for proving spontaneous magnetization in the classical Heisenberg model; its difficult extension to quantum systems was done in [12]. The claims of [12, 20] that are relevant here deal with spontaneous magnetization in the spin-$\frac{1}{2}$ x-y model. Let us discuss analogies between spins and hard-core boson systems. For the latter, we take $\mathcal{H}_0 \simeq \mathbb{C}^2$ and define self-adjoint operators $\{S_x^{(1)}, S_x^{(2)}, S_x^{(3)}\}_{x\in\mathbb{Z}^d}$, that commute if they are located on different sites, and satisfy $[S_x^{(1)}, S_x^{(2)}] = \mathrm{i}S_x^{(3)}$ (and cycle permutations of (1,2,3)) at a same site x. The x-y model has interaction $-S_x^{(1)}S_y^{(1)} - S_x^{(2)}S_y^{(2)}$ on nearest-neighbor sites x, y, and zero otherwise.

The correspondence to boson models is done by setting

$$\begin{aligned} c_x^\dagger &= S_x^{(1)} + \mathrm{i}S_x^{(2)} \\ c_x &= S_x^{(1)} - \mathrm{i}S_x^{(2)} \\ n_x &= S_x^{(3)} + \tfrac{1}{2}. \end{aligned} \tag{5.4}$$

In the case of hard-cores (with $N = 1$) the commutation relations are $[c_x^\#, c_y^\#] = 0$ if $x \neq y$, and $\{c_x, c_x^\dagger\} = 1$, where $\{\cdot,\cdot\}$ denotes the anticommutator. It is easy to check that these also follow from the commutation relations of spin operators, and from definitions above. The x-y model is equivalent to H',

$$H'_A = \begin{cases} -\frac{1}{2}[c_x^\dagger c_y + c_y^\dagger c_x] & \text{if } A = \{x, y\}, \quad |x-y| = 1 \\ 0 & \text{otherwise.} \end{cases} \tag{5.5}$$

Off-diagonal long-range order is then equivalent to spontaneous magnetization in the 1-2 plane.

The hard-core model was the object of an original study by Sütő. By the Perron–Frobenius theorem, the ground state can be chosen with positive coefficients. This induces a probability measure on the space of configurations, and one can show that this measure is concentrated on those configurations with a special density of pairs (0,1). See [34].

5.4 BEC & symmetry breaking

The Bose–Einstein condensation is related to a symmetry breaking, namely of 'global gauge invariance'. Let us note that the Hamiltonian (3.1) conserves the total number of particles, i.e.,

$$\big[\sum_{A\subset\Lambda} H_A, \sum_{x\in\Lambda} \hat{n}_x\big] = 0. \tag{5.6}$$

Therefore one can define the unitary operator $U_\Lambda = \mathrm{e}^{\mathrm{i}\alpha \sum_{x\in\Lambda} \hat{n}_x}$, which is a symmetry of the Hamiltonian. Its action on creation and annihilation operators is

$$\begin{aligned} U_\Lambda c_x^\dagger U_\Lambda^{-1} &= \mathrm{e}^{\mathrm{i}\alpha}\, c_x^\dagger \\ U_\Lambda c_x U_\Lambda^{-1} &= \mathrm{e}^{-\mathrm{i}\alpha}\, c_x^\dagger. \end{aligned} \tag{5.7}$$

This is easily seen from the action of all these operators on elements of the basis (2.1).

To study the properties of the free energies as a function of the interactions, one has to proceed as in Section 3. Recall that we added a non translation-invariant (and non-physical) interaction hP and looked at a phase diagram where h is a parameter. This is similar here. First, we need an interaction that does not conserve the total number of particles. The simplest choice with self-adjoint operators is $Q = (Q_A)$, with

$$Q_A = \begin{cases} \mathrm{e}^{\mathrm{i}\alpha}\, c_x^\dagger + \mathrm{e}^{-\mathrm{i}\alpha}\, c_x & \text{if } A = \{x\} \\ 0 & \text{otherwise.} \end{cases} \tag{5.8}$$

Supposedly, there is a unique tangent functional to the free energy at $H + hQ$ for all $h \neq 0$, but there should be an infinite number of extremal states at $h = 0$ (if the temperature is low enough); each of these extremal states is indexed by $\alpha \in [0, 2\pi)$. Since there is a unique equilibrium state at high temperature (Theorem 3.1), we face here the breakdown of a continuous symmetry. It should occur at low temperature and if the dimension of the lattice is greater or equal to 3.

There is no rigorous result to support this discussion, besides the weaker — but important! — statement of Theorem 5.1 in the case of the hard-core boson gas.

6 Infinite Cycles: Context and Conjectures

6.1 Heuristics

In the last section of this brief review, we discuss an approach to the BEC initiated by Feynman 50 years ago [13], that focusses on the occurrence of infinite cycles in the space-time representation. Its appeal to probabilists should be evident — it looks at first sight like a percolation phenomenon. However, the one-dimensional nature of cycles makes them harder to study than clusters. Still, some progress should be possible.

The partition function for the Hamiltonian (5.1) can be expanded via the

Feynman–Kac formula; setting $\hbar^2/2m = 1$; the partition function is given by

$$Z_V = \sum_{N \geqslant 0} \frac{\mathrm{e}^{\beta\mu N}}{N!} \int_V \mathrm{d}x_1 \dots \mathrm{d}x_N \sum_{\pi \in S_N} \Big(\prod_{i=1}^{N} \int_{\substack{\boldsymbol{x}_i(0)=x_i \\ \boldsymbol{x}_i(\beta)=x_{\pi(i)}}} \mathrm{d}W_{[0,\beta]}(\boldsymbol{x}_i) \Big) \exp\Big\{ - \int_0^\beta \mathrm{d}\tau \sum_{i<j} U(|\boldsymbol{x}_i(\tau) - \boldsymbol{x}_j(\tau)|) \Big\}. \quad (6.1)$$

Here, integrals are over Brownian paths starting at x_i and ending at $x_{\pi(i)}$. An introduction to functional integration can be found in [17]. This expression is very similar to (4.6) for lattice systems and is illustrated in Fig. 6.

The space-time is periodic in the vertical direction, so it is topologically equivalent to a cylinder. Bosons wind around the cylinder, forming cycles (see Fig. 6). Feynman's idea is to consider the length of these cycles, and to look at the probability of occurrence of infinite ones. He identifies the onset of a positive probability to a Bose–Einstein condensation. In his paper [13] he argues that interactions only slow down the diffusion of bosons, without forbidding infinite cycles, and he concludes that BEC should also occur in interacting systems.

Cycles were studied in [33], where it is proved in particular that, in the case of the ideal gas (that is, non-interacting particles), infinite cycles do occur below the transition temperature for BEC.

However, the equivalence between BEC and occurrence of infinite cycles is not obvious. Consider e.g., the model discussed in Section 3. Our results imply absence of BEC at low temperature and with small T; on the other hand, even though they have restricted motions, bosons can interchange with neighbors, and infinite cycles seem likely for low enough temperature, if the dimension is greater than or equal to 3 — this has something to do with probabilities of recurrence of random walks. A configuration of a lattice model can be viewed as a configuration of a continuum model where the particles have condensed (in

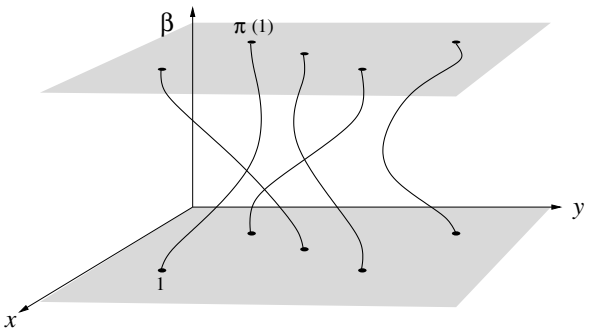

Figure 6. Feynman–Kac representation of the partition function for bosons in the continuum. The picture shows a situations with five particles and two cycles, of lengths 4 and 1.

the usual sense) and are displaying long-range order. The following conjecture is compatible with these considerations:

Conjecture.

- *Occurrence of BEC implies positive probability of infinite cycles.*
- *Positive probability of infinite cycles, and absence of long-range order, imply occurrence of BEC.*

In the hope of shedding some light on this discussion, we introduce a simple lattice model of cycles, state some (rather obvious) properties and propose some conjectures.

6.2 A simple lattice model of cycles

The expression (6.1) for the partition function starts by an integration over all initial positions of the particles. Let us suppose that they are located on the sites of the lattice $\mathbb{Z}^d$ — assuming that density fluctuations do not play an important role in BEC, this assumption is a mild one at low temperature. Furthermore, we replace the integral over Brownian paths by an effective weight

$$\prod_{x\in\Lambda} \mathrm{e}^{-\xi(x,\pi(x))}$$

(with $\Lambda \subset \mathbb{Z}^d$ finite). A natural choice for $\xi(x,y)$ is $|x-y|^2/\beta$, with $|\cdot|$ the Euclidian distance, and β the inverse temperature. Indeed, the Brownian paths for a time interval $[0,\beta]$ diffuse like $\sqrt{\beta}$. Other choices are possible, for instance $|x-y|^\gamma/\beta$ with $\gamma > 2$ to account for large interactions. One could also simplify the problem and consider

$$\xi(x,y) = \begin{cases} 0 & \text{if } x = y \\ 1/\beta & \text{if } |x-y| = 1 \\ \infty & \text{otherwise.} \end{cases} \tag{6.2}$$

In any case, we restrict the choice of ξ to one that satisfies

$$\sum_x \mathrm{e}^{-\xi(0,x)} < \infty, \tag{6.3}$$

ensuring that particles do not jump to infinity in one step.

Let us describe carefully these models of cycles.

The lattice is $\mathbb{Z}^d$, and we denote by $\mathbb{B}$ the set of bijections $\mathbb{Z}^d \to \mathbb{Z}^d$. Given $x, y \in \mathbb{Z}^d$, let $B_{xy} = \{\pi \in \mathbb{B} : \pi(x) = y\}$; then we define $\mathcal{B}'$ to be the algebra made out of all such sets and their complements.

Next we set $\mathbb{B}(\Lambda) = \{\pi \in \mathbb{B} : \pi(x) = x \text{ for all } x \notin \Lambda\}$ the set of permutations that are trivial outside Λ. Since $\mathcal{B}'$ is countable, there exists a sequence of

increasing boxes $\mathbf{\Lambda} = (\Lambda^{(n)})_{n \geqslant 0}$ such that for all $B \in \mathcal{B}'$ the following limit exists:

$$P(B) = \lim_{\Lambda \in \mathbf{\Lambda}} P_\Lambda(B), \tag{6.4}$$

with

$$P_\Lambda(B) = \frac{1}{Z(\Lambda)} \sum_{\pi \in \mathbb{B}(\Lambda)} \mathbb{I}\left[\pi \in B\right] \prod_{x \in \Lambda} \mathrm{e}^{-\xi(x,\pi(x))}. \tag{6.5}$$

The normalization $Z(\Lambda)$ is

$$Z(\Lambda) = \sum_{\pi \in \mathbb{B}(\Lambda)} \prod_{x \in \Lambda} \mathrm{e}^{-\xi(x,\pi(x))}. \tag{6.6}$$

The probability (6.4) extends to the smallest σ-algebra generated by $\mathcal{B}'$, which we denote $\mathcal{B}$.

A *cycle* is a sequence $c = (x_1, \ldots, x_{|c|})$ of different sites; we identify

$$(x_2, \ldots, x_{|c|}, x_1) = (x_1, \ldots, x_{|c|}).$$

The set of permutations $B_c = \{\pi \in \mathbb{B} : \pi(x_j) = x_{j+1}, 1 \leqslant j \leqslant n\}$ (with $x_{|c|+1} \equiv x_1$) is an element of $\mathcal{B}$, and the set of cycles is countable. Therefore, the set

$$B_\infty = \mathbb{B} \setminus \bigcup_{c \ni 0} B_c \tag{6.7}$$

is also in the σ-algebra $\mathcal{B}$. It represents the event 'the origin belongs to an infinite cycle', and is the central object of our attention.

6.3 Few results and important conjectures

There are no infinite cycles at high temperature; the condition of the following theorem is easy to check for small β.

Theorem 6.1. *If*

$$\sum_{c \ni 0} \prod_{j=1}^{|c|} \mathrm{e}^{-\xi(x_j, x_{j+1})} < \infty,$$

then $P(B_\infty) = 0$.

Proof. Let $B_{>n}$ be the set of permutations where the origin belongs to a cycle of length greater than n. One has

$$B_{>1} \supset B_{>2} \supset \cdots \quad \text{and} \quad B_\infty = \bigcap_n B_{>n}. \tag{6.8}$$

Then $P(B_\infty) = \lim_n P(B_{>n})$. Since

$$B_{>n} = \bigcup_{x \neq 0} \bigcup_{\substack{w: 0 \to x \\ |w| = n}} B_w, \tag{6.9}$$

with $w = (0, x_1, \dots, x_{n-1}, x)$ a self-avoiding walk from 0 to x, and $B_w = \cap_{j=1}^n B_{x_{j-1}, x_j}$, one can write

$$\begin{aligned} P(B_{>n}) &= \sum_{x \neq 0} \sum_{\substack{w: 0 \to x \\ |w| = n}} \lim_{\Lambda \in \mathbf{\Lambda}} P_\Lambda(B_w) \\ &\leqslant \lim_{\Lambda \in \mathbf{\Lambda}} \sum_{x \neq 0} \sum_{\substack{w: 0 \to x \\ |w| = n}} P_\Lambda(B_w) \\ &= \lim_{\Lambda \in \mathbf{\Lambda}} \sum_{\substack{c \ni 0 \\ |c| > n}} \prod_{j=1}^{|c|} \mathrm{e}^{-\xi(x_{j-1}, x_j)} \, \frac{Z(\Lambda \setminus c)}{Z(\Lambda)} \\ &\leqslant \sum_{\substack{c \ni 0 \\ |c| > n}} \prod_{j=1}^{|c|} \mathrm{e}^{-\xi(x_{j-1}, x_j)} \, . \end{aligned}$$

The first inequality is Fatou's lemma. The last term goes to 0 as $n \to \infty$ since the sum over all cycles containing the origin converges. □

The typical picture at high temperature is that of Fig. 7 (a). Most cycles involve a unique site and have length 1. When the temperature decreases, the lengths of the cycles should increase, as depicted in Fig. 7 (b).

The model of cycles is a model of self-avoiding closed random walks (random polygons), that cover the lattice and interact via mutual exclusion. One is interested in the walk that contains the origin, for which one can write a probability

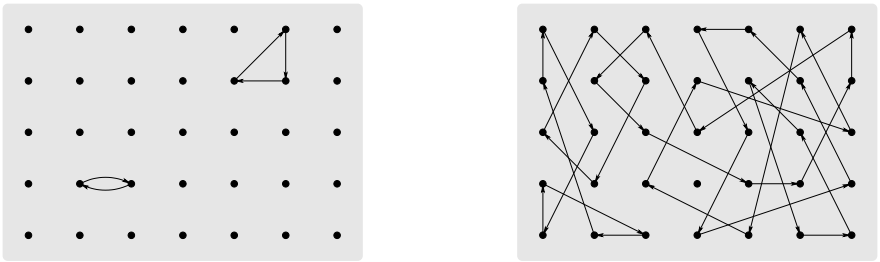

Figure 7. Expected typical configurations of cycles, (a) at high temperature and (b) at low temperature.

distribution. It may resemble the probability distribution for random polygons, but not exactly: other walks need to breathe and exert a pressure on the walk containing the origin. Let us assume however that both probability distributions are qualitatively similar. The probability for the occurrence of an infinite cycle is then related to the recurrence or the transcience of random walks. It is actually known that the random walk is recurrent in dimension 2 and transcient in dimension 3 and higher. One then expects infinite cycles to appear in dimensions larger or equal to 3, and at low temperature. This illustrates the effect of the dimension in the onset of Bose–Einstein condensation.

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