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Low-Density Expansion for Unstable Interactions and a Model of Crystallization

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For a class of unstable pair interactions in classical continuous systems of identical particles the high-temperature thermodynamic behavior is shown to be normal by extending low-density theorems for the correlation functions. In an example we prove a transition between a translation-invariant phase at high temperatures and low densities and a solid with long-range order at low temperatures. The transition is "catastropic" in the sense that it is accompanied by the divergence of thermodynamic quantities. We also exhibit counterexamples of unstable interactions in any dimension which do not give rise to a low-temperature catastrophe.

KEY WORDS: Continuous system; unstable interaction; cluster expansion; crystal.

1. INTRODUCTION

Expansions of thermodynamic quantities in powers of the density or the activity provide a powerful tool to study systems of particles on a lattice or in the continuum. The convergence of such expansions, such as the virial and Mayer expansions or the power series of correlation functions, indicates the absence of phase transitions and was the subject of many rigorous works in the 1960s and 1970s (e.g., refs. 17, 18, 8, 9, 20, 13, 14, 4, 5, and 10). Convergence was shown for stable regular pair interactions under the condition that the activity or the density is sufficiently small.

Stability ensures that the energy of the ground state is an extensive quantity, a condition which is not always satisfied, the most remarkable

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exceptions being the Coulomb and gravitational interactions. The extension of convergence theorems to unstable interactions has long been an important task, successfully attacked in several cases (see Brydges[3] for a recent review). In this paper Ruelle's treatment[20] will be extended and discussed through examples which include a model of crystallization.

Crystallization is an everyday phenomenon whose microscopic description is very far from being satisfactory. Phrased in terms of statistical physics, the problem consists in proving that in continuous space a system of particles with translation-invariant interaction energy undergoes a phase transition at a positive temperature, during which the invariance under translation of the equilibrium state is broken.

The few rigorous results are valid in low (one or two) dimensions. In general, proving that the ground state is periodic (or quasiperiodic) is already a hard problem.[19] It is known, due to Mermin[15] (see also Fröhlich and Pfister[7]) that in one- and two-dimensional systems with stable regular pair potentials which are smooth outside the origin the equilibrium state is translation invariant at any positive temperature. The one-dimensional, one-component plasma, when treated classically, is in a crystalline state at any positive temperature[12] and its quantum mechanical ground state is also ordered.[2] In lattice systems we know phase transitions which break translation invariance; the simplest example is provided by the antiferromagnetic Ising model. Other, more complicated interactions can lead to quasiperiodic order.[16] The low-temperature order found by Kennedy and Lieb[11] in the Falicov–Kimball model can also be interpreted as a crystalline order. However, to my knowledge, there exists no example of a proof that a particle system in continuous space exhibits a transition from fluid to an ordered solid at a positive temperature.

The present paper will provide such an example, even though a caricatural one. In general, the main difficulties of a rigorous treatment of crystallization are in the poor knowledge of the ground state and in dealing with the continuous excitations. We circumvent these problems by choosing an unstable interaction which forces the particles to settle down into well-defined relative positions with respect to each other already at a positive temperature. The difficulty is then shifted elsewhere: to the proof that at high temperatures the system has a normal thermodynamic behavior, including the absence of ordering.

We will study systems of identical particles evolving in the D-dimensional Euclidean space $\mathbf{R}^D$ and interacting via a classical translation-invariant pair interaction: For x_i, x_j in $\mathbf{R}^D$,

$$\phi(x_i, x_j) = \phi_{b,\alpha}(x_j - x_i)$$

and

$$\phi_{b,\alpha} = \begin{cases} +\infty & \text{if } |x| < a \\ -b_k^{-\mu} & \text{if } b_k - \alpha_k < |x| < b_k + \alpha_k, \quad k = 1, 2, \ldots \\ 0 & \text{otherwise} \end{cases} \tag{1.1}$$

Here $a > 0$ is the hard-core diameter and $\mu \leqslant D$ ($\mu < 0$ is allowed). The sequence b_k is positive, increasing, and tends to infinity, $b_1 > a$. The α_k are positive and so determined that the intervals which appear in the definition of $\phi_{b,\alpha}$ are nonoverlapping. One may think of $\phi_{b,\alpha}$ as a regularized imitation of nonregular oscillating-decaying interactions like, e.g., the RKKY one.

The family of interactions for which the phase transition will be shown corresponds to $D = 1$, $b_k = k$, and

$$\alpha_k = \begin{cases} ck^{-\nu} & \text{if } \mu = 1 \\ c^{k^{1-\mu}} & \text{if } \mu < 1 \end{cases} \tag{1.2}$$

In this formula $\nu > 1$, and the condition to have nonoverlapping intervals entails $a \leqslant 1 - 2c$. We will also suppose $2c < a$ (so $c < 1/4$), which simplifies the description of the ground states. In both cases ($\mu = 1$ and $\mu < 1$) the family of interactions is parametrized by three continuous parameters (a, c, ν and a, c, μ, resp.), two of which (a and c) are of less importance. The letter φ will refer to a member of this family. φ is manifestly unstable: The potential energy of N particles in the configuration $x_i = i$, $i = 1, \ldots, N$, is

$$\begin{aligned} U(x)_N &= \sum_{1 \leqslant i < j \leqslant N} \varphi(x_j - x_i) = -\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (j-i)^{-\mu} = -\sum_{n=1}^{N-1} \frac{N-n}{n^\mu} \\ &\equiv E_\mu(N) \asymp \begin{cases} -N \ln N & \text{if } \mu = 1 \\ -\dfrac{N^{2-\mu}}{(1-\mu)(2-\mu)} & \text{if } \mu < 1 \end{cases} \end{aligned} \tag{1.3}$$

The last term gives the leading order in N as N goes to infinity. Thus, the stability condition,

$$U(x)_N \geqslant -BN \tag{1.4}$$

with some finite B independent of N and $(x)_N$, is not fulfilled. Here and below we use the shorthand $(x)_N = (x_1, \ldots, x_N)$. By cutting windows of widths $2\alpha_k$ and permitting the attraction to act only at distances which fall into these windows we can at will decrease the domain of the configuration space in which the potential energy is nonextensive. With a suitable tuning of the windows—precisely as in (1.2)—we will get a phase transition. The upshot is that in the limit of infinite volume the Gibbs measure of the domain of nonextensivity tends to zero at high temperature and to a positive value at low temperature. This latter implies a catastrophe in the infinite system. Something similar happens in the two-dimensional Yukawa gas[1] (see also ref. 6), but now the catastrophe does not manifest itself in a mere collapse. Instead, the particles get stuck in positions of a periodic lattice of period 1. This is accompanied by the divergence of thermodynamic quantities: The free energy per particle goes to $-\infty$, the grand-canonical potential—and the grand-canonical pressure with it—to $+\infty$. Notice that for a hard-core repulsion and the one-dimensional RKKY interaction $-\cos 2\pi x/|x|$ outside the hard core one gets this kind of divergence at all temperatures.

While it is very simple to show that at low temperatures φ gives rise to diverging thermodynamic quantities, the proof of the long-range order is more complicated. Also, a direct proof that the pressure remains bounded at high temperatures can be done, but showing directly the analyticity, translation invariance, and clustering of the correlation functions seems to be prohibitive. These properties will follow from our extension of the treatment of correlation functions via the Kirkwood–Salsburg equation or the algebraic method, as described in Ruelle's book.[20] The condition of stability shall be relaxed. The price to pay is to replace the regularity condition by a stronger one [condition (C) below] which may not be satisfied at all temperatures.

The interactions $\phi_{b,\alpha}$ emerge as natural examples satisfying (C). Indeed, we shall see that for any choice of the sequence b_k the α_k can be chosen so that (C) holds true. Now (C) will imply the boundedness of the pressure and, for low activities, the expected properties of the correlations.

All the results remain obviously valid if we define $\phi_{b,\alpha} = -|x|^{-\mu}$ inside the windows. Also, the interaction can be made continuous, although with unbounded derivative. The one-dimensional example of phase transition can somewhat be extended: for instance, we get qualitatively the same result if b_k is any sequence of integers such that $b_{k+1} - b_k$ is a bounded sequence.

To obtain examples in higher dimension, one has to find b_k and α_k so that (C) holds at small inverse temperatures β and there is a catastrophe at large β. As will be seen, checking (C) is straightforward; finding the ground states or configurations with nonextensive energy is more involved. For the natural choice $b_k = k$ the suitable α_k seem not to exist. More artificial choices for b_k, such as, for example, the kth neighbor distance on a lattice, can work. Also, with a nonisotropic interaction, where there are attractive windows only at lattice vectors corresponding to some lattice, one can easily obtain this kind of phase transition.

The paper is organized as follows. Section 2 contains our extension of convergence theorems for high temperatures and low activities. We prove that the high-temperature thermodynamic behavior of a classical system of identical particles in $\mathbf{R}^D$ is "normal" if the interaction satisfies the following condition:

(C) ϕ is a translation- and reflection-invariant pair interaction,

$$\phi(x, y) = \phi(y - x) = \phi(x - y)$$

which can be decomposed as $\phi = \phi_1 + \phi_2$, where ϕ_2 is stable and

$$C(\beta) = \sup_{n, (x)_n : U_1(x)_n < \infty} \int |e^{-\beta\phi(y)} - 1| \exp\left\{-\beta \sum_{i=1}^{n} \phi_1(y - x_i)\right\} dy < \infty$$

for some $\beta > 0$. Here U_1 is the potential energy corresponding to ϕ_1.

This condition may not be satisfied for all β, but if it holds for some $\beta_0 > 0$, it holds also for $\beta < \beta_0$. If ϕ is stable, one can set $\phi_1 = 0$ and (C) reduces to the regularity condition. We will see that an unstable interaction satisfying (C) must contain a hard core: this excludes the instability due to $\phi(0) < 0$. We prove that all the results on the correlation functions described in Chapter 4 of ref. 20 remain valid if Ruelle's $C(\beta)$ and B are replaced, respectively, by the $C(\beta)$ above and the stability bound of U_2, the potential energy belonging to ϕ_2. Under the additional condition that (C) holds with $\phi = \phi_1$ the boundedness of the pressure is shown for all activities.

In Section 3 we study the interactions $\phi_{b,\alpha}$. We show that for any choice of b_k, condition (C) can be satisfied if α_k is sufficiently rapidly decaying. The α_k can even be fixed so that (C) holds for any positive temperature: this will provide examples of unstable interactions which do not give rise to a catastrophe at low temperature. The one-dimensional interaction φ specifying the model of crystallization will be seen to satisfy (C) with $\phi = \phi_1 = \varphi$ for $\beta < (\nu - 1)/2$ if $\mu = 1$ and for $\beta < \frac{1}{2}(1 - \mu) \ln(1/c)$ if $\mu < 1$.

In Section 4 we describe the low-temperature properties of the model of crystallization. We briefly discuss the ground states, which can be quite interesting for $\mu < 0$, and present a nonrigorous energy-entropy argument predicting the phase transition. The low-temperature catastrophe (in the sense of the divergence of the specific free energy or the grand-canonical pressure) is established for $\beta > \nu$ in the case $\mu = 1$ and for $\beta > (1 - \mu)(2 - \mu) \ln(1/c)$ in the case $\mu < 1$. The thresholds are the same as those found with the nonrigorous argument. In the same temperature domain we show the existence of nondecaying pair correlations. Our proof of ordering is incomplete: We prove that particles are at integer distances, occupying some positions of a lattice of period 1 (say, $\mathbf{Z}$), but cannot say anything about the arrangement *within* this lattice. One may expect that for $\mu > 0$ and the density $\rho < 1$, there is phase separation between a period-1 lattice and a "phase" of density 0, while for $\mu < 0$ and $\rho < 1$ the arrangement is lacunary and depends on the density: if ρ is rational, the particles occupy some periodic sublattice; if ρ is irrational, there is some quasiperiodic order.

2. CORRELATIONS AND PRESSURE AT HIGH TEMPERATURES FOR A CLASS OF UNSTABLE INTERACTIONS

2.1. Definitions, Notations, and Classical Results

We consider a collection of identical particles in bounded Lebesgue-measurable D-dimensional domains Λ, interacting via a translation-invariant pair interaction ϕ. We will extend some results on the infinite-volume limit of correlation functions at high temperatures and low activities. Recall that the m-point correlation function in the canonical ensemble is defined by

$$\rho_{\Lambda,N}(x)_m = N(N-1)\cdots(N-m+1)\,\chi_\Lambda(x)_m \times \frac{\int_{\Lambda^{N-m}} d(y)_{N-m} \exp[-\beta U((x)_m \cup (y)_{N-m})]}{\int_{\Lambda^N} d(y)_N \exp[-\beta U(y)_N]} \tag{2.1}$$

with

$$\chi_\Lambda(x)_m = \chi_\Lambda(x_1)\cdots\chi_\Lambda(x_m) \tag{2.2}$$

where $\chi_\Lambda(x)$ is the characteristic function of Λ and

$$U(x)_N = \tfrac{1}{2}\sum_{i\neq j} \phi(x_j - x_i) \tag{2.3}$$

If the x_i are all different, $\rho_{\Lambda,N}(x)_m$ is the canonical average [over $(y)_N$] of

$$\prod_{i=1}^{m} \sum_j \delta(x_i - y_j)$$

Notice that $\sum_j \delta(x - y_j)$ is the particle density observable.

Denote $Q_{\Lambda,N}$ and Ξ_Λ the canonical and grand-canonical partition functions, respectively:

$$Q_{\Lambda,N}=\frac{1}{N!}\int_{\Lambda^N} e^{-\beta U(x)_N}\, d(x)_N \tag{2.4}$$

and

$$\Xi_\Lambda=\sum_{n\geqslant 0} z^n Q_{\Lambda,n} \tag{2.5}$$

where z is the activity or fugacity. (More precisely, $z=e^{\beta\mu_c}/\lambda_{\mathrm{B}}^D$, where μ_c is the chemical potential and λ_{B} is the thermal de Broglie wavelength. As usual, we consider z instead of μ_c as an independent variable.) The grand-canonical quantity corresponding to $\rho_{\Lambda,N}$ is

$$\begin{aligned}\rho_\Lambda(x)_m&=\sum_{n\geqslant 0} z^n Q_{\Lambda,n}\rho_{\Lambda,n}(x)_m \Big/ \sum_{n\geqslant 0} z^n Q_{\Lambda,n}\\ &=\Xi_\Lambda^{-1} z^m \chi_\Lambda(x)_m \sum_{n\geqslant 0}\frac{z^n}{n!}\int_{\Lambda^n} d(y)_n\, e^{-\beta U((x)_m\cup(y)_n)}\end{aligned} \tag{2.6}$$

where we used that $\rho_{\Lambda,n}(x)_m=0$ if $m>n$.

The normalization of the correlation function allows $\rho_\Lambda(x)_m$ to have a finite nonvanishing limit $\rho(x)_m$ when Λ increases to $\mathbf{R}^D$. The same is true for $\rho_{\Lambda,N}(x)_m$ if the limit is performed with the density $N/|\Lambda|$ fixed. These limits are expected to exist at high temperatures and low densities or activities when any "not too strongly" interacting system "resembles" a system of free particles. Correlation functions can be used to make precise what this resemblence means:

(i) Existence of the above-mentioned limits, i.e., their independence of the way Λ tends to $\mathbf{R}^D$.

(ii) Translation invariance of each correlation function,

$$\rho(x_1+x,\dots,x_m+x)=\rho(x_1,\dots,x_m) \tag{2.7}$$

for every x_i, $x\in\mathbf{R}^D$, without which the equilibrium state in infinite volume would not be unique.

(iii) Mixing or cluster property, characterizing the asymptotic independence of the particles. In its weakest form this states that for any two groups $(x)_m$ and $(y)_n$ of positions

$$\rho(x_1,\dots,x_m,y_1,\dots,y_n)-\rho(x)_m\,\rho(y)_n\to 0 \quad \text{if}\quad |x_i-y_j|\to\infty,\qquad \text{all}\quad i,j \tag{2.8}$$

There is a series of classic results on lattice and continuous systems cited in the Introduction and partly resumed in ref. 20, proving among others the above properties. Because of the explicit dependence on z, ρ_Λ is easier to deal with than $\rho_{\Lambda,N}$. All the methods consider $\rho_\Lambda(x)_m$ as a function of the activity and extend it to complex values of z. It is then proved, using the Kirkwood–Salsburg equation or some kind of cluster expansion, that all these functions have a common domain of analyticity in z, depending on β but not on Λ, m, and $(x)_m$. Inside this domain every $\rho_\Lambda(x)_m$ converges with Λ tending to $\mathbf{R}^D$ to an analytic function $\rho(x)_m$ which is translation invariant, and the different functions are related through the mixing property.

These results are derived for stable regular pair interactions. Stability was defined in Eq. (1.4). A translation-invariant pair interaction ϕ is called *regular* if it is bounded below and

$$\int_{|y|>r} |\phi(y)| \, dy < \infty$$

for some finite r. If ϕ is bounded below, it is regular if and only if

$$\tilde{C}(\beta) = \int |e^{-\beta\phi(y)} - 1| \, dy < \infty \tag{2.9}$$

for some (and, hence, all) $\beta > 0$. This can be seen by choosing r so that $|\phi(y)| < 1$ for $|y| > r$. For stable regular pair interactions the analyticity of the correlation functions and properties (i)–(iii) are shown for complex values of z in the disk

$$|z| < (e^{2\beta B + 1} \tilde{C}(\beta))^{-1} \tag{2.10}$$

(see ref. 20). Notice that with increasing β the domain of analyticity diminishes but never disappears.

2.2. Correlation Functions for Unstable Interactions

Extensions of the above results to unstable interactions have been motivated mainly by the interest in systems of charged particles (reviewed in ref. 3). The technique is much more involved than ours; yet, it does not seem to be adapted to deal with the "infrared" instability characterizing the interactions (1.1). The following theorem offers an extension to this direction.

Theorem 1. Let ϕ be a pair interaction satisfying condition (C) at a given $\beta>0$, B a real constant defined through $U_2(x)_n \geqslant -Bn$, and

$$D_\beta = \{z \in \mathbf{C}: |z| < (e^{2\beta B+1} C(\beta))^{-1}\} \tag{2.11}$$

For every bounded Lebesgue measurable $\Lambda \subset \mathbf{R}^D$, $\Xi_\Lambda(z)$ has no zeros in D_β and for every positive integer m and $(x)_m \in \mathbf{R}^{mD}$, $\rho_\Lambda(x)_m$ is an analytic function of z in D_β. Now,

$$\rho(x)_m = \lim_{\Lambda \to \mathbf{R}^D} \rho_\Lambda(x)_m$$

exists, it is analytic inside D_β, and it is translation invariant; in particular, $\rho(x)_1 \equiv \rho(x_1)$ is constant. Mixing holds in the form (2.8).

Condition (C) has several interesting implications.

1. Clearly, $C(\beta)<\infty$ implies $\tilde{C}(\beta)<\infty$. Therefore, if ϕ is bounded below, it is regular.

2. If $C(\gamma)<\infty$ for some $\gamma>0$, $C(\beta)<\infty$ for any $\beta<\gamma$. To see this, notice that $|e^{-\beta\phi(y)}-1|$ increases with increasing β; therefore, with

$$W_1(y,(x)_n) = \sum_{i=1}^{n} \phi_1(y-x_i) \tag{2.12}$$

one obtains

$$\begin{aligned}
&\int |e^{-\beta\phi(y)}-1|\, e^{-\beta W_1(y,(x)_n)}\, dy \\
&\quad = \int_{W_1>0} |e^{-\beta\phi(y)}-1|\, e^{-\beta W_1}\, dy + \int_{W_1\leqslant 0} |e^{-\beta\phi(y)}-1|\, e^{-\beta W_1}\, dy \\
&\quad \leqslant \int_{W_1>0} |e^{-\gamma\phi(y)}-1|\, dy + \int_{W_1\leqslant 0} |e^{-\gamma\phi(y)}-1|\, e^{-\gamma W_1}\, dy \leqslant 2C(\gamma)
\end{aligned} \tag{2.13}$$

Taking the supremum, we get $C(\beta)\leqslant 2C(\gamma)$. In fact, $C(\beta)\to 0$ as $\beta\to 0$. If $\phi_1\leqslant 0$ (outside, perhaps, a hard core), the integral for $W_1>0$ can be dropped, implying that $C(\beta)$ is a monotonically increasing function of β.

3. If ϕ is stable, one can set $\phi_1=0$ and (C) reduces to the regularity condition. If ϕ is unstable and satisfies the condition, it must have a hard core. More precisely, the following holds.

Proposition 1. Let ϕ satisfy (C) and suppose there exists an open set $V\subset\mathbf{R}^D$ and $\varepsilon_1, \varepsilon_2>0$ such that $\phi_1(x)\leqslant -\varepsilon_1$, $|\phi(x)|\geqslant\varepsilon_2$ if $x\in V$. Then $\phi_1(x)=\infty$ [and hence $\phi(x)=\infty$] if $|x|<a$ for some $a>0$.

Proof. Assume that the conditions of the proposition hold true, yet ϕ_1 has no hard core. Then for any $\eta > 0$ there is an infinite set $X_\eta \subset \mathbf{R}^D$ such that $|x| < \eta$ for $x \in X_\eta$ and $\phi_1(x-y) < \infty$ for $x, y \in X_\eta$. Choose an open set $V_0 \subset V$ with $\operatorname{dist}(V_0, V^c) > \eta_0$; such an $\eta_0 > 0$ exists. Let $(x)_n \subset X_{\eta_0}$. Then $U_1(x)_n < \infty$ and $y - x_i \in V$ for $y \in V_0$. It follows that

$$\begin{aligned} a_n &= \int |e^{-\beta\phi(y)} - 1|\, e^{-\beta W_1(y,(x)_n)}\, dy \\ &\geqslant \int_{V_0} |e^{-\beta\phi(y)} - 1|\, e^{-\beta W_1(y,(x)_n)}\, dy \\ &\geqslant |V_0|\, e^{n\beta\varepsilon_1} \min\{e^{\beta\varepsilon_2} - 1, 1 - e^{-\beta\varepsilon_2}\} \end{aligned} \tag{2.14}$$

so the sequence $\{a_n\}$ is unbounded for any $\beta > 0$, contradicting (C). ∎

Proof of Theorem 2. We use the algebraic method of cluster expansion as described in ref. 20. For definitions and the properties of the underlying algebra $\mathscr{A}$ of function sequences the reader is referred to that book.

The starting point is to rewrite ρ_Λ in the form of a power series in z:

$$\rho_\Lambda(x)_m = z^m \chi_\Lambda(x)_m \sum_{n=0}^{\infty} \frac{z^n}{n!} \int d(y)_n\, \chi_\Lambda(y)_n\, \psi_{(x)_m}(y)_n \tag{2.15}$$

where

$$\psi_{(x)_m}(y)_n = ((e^{-\beta U})^{-1} * D_{(x)_m} e^{-\beta U})(y)_n \tag{2.16}$$

Here $*$ is the multiplication and $D_{(x)_m}$ is the derivation in $\mathscr{A}$,

$$e^{-\beta U} = (e^{-\beta U(x)_n})_{n \geqslant 0} \tag{2.17}$$

is the sequence of Boltzmann factors and $(e^{-\beta U})^{-1}$ is its inverse in $\mathscr{A}$. The zeroth term of the sum in (2.15) is $(\psi_{(x)_m})_0 = e^{-\beta U(x)_m}$. One can write $e^{-\beta U}$ and its inverse as

$$e^{-\beta U} = \operatorname{Exp} u, \qquad (e^{-\beta U})^{-1} = \operatorname{Exp}(-u) \tag{2.18}$$

where Exp is the exponential in $\mathscr{A}$ and $u = (u(x)_n)_{n \geqslant 0}$ is the sequence of Ursell functions. ψ is the same as $\tilde{\varphi}$ in ref. 20.

If $(x)_m$ is an illicit configuration, i.e., $U(x)_m = \infty$, then, according to Eq. (2.6), $\rho_\Lambda(x)_m = 0$. We will show that under condition (C),

$$\begin{aligned} \Psi_n(x)_m &= \int d(y)_n\, |\psi_{(x)_m}(y)_n| \\ &\leqslant n!\, C(\beta)^n \exp[-\beta U_1(x)_m + (2\beta B + 1)(m+n-1)] \end{aligned} \tag{2.19}$$

for $n \geqslant 0$, $m \geqslant 1$, and any admissible configuration $(x)_m$ [i.e., such that $U_1(x)_m < \infty$].

Let us suppose for the moment that (2.19) holds true. Then

$$\begin{aligned}
&\left| \sum_{n=0}^{\infty} \frac{z^n}{n!} \int d(y)_n \chi_A(y)_n \psi_{(x)_m}(y)_n \right| \\
&\quad \leqslant \sum_{n=0}^{\infty} \frac{|z|^n}{n!} \Psi_n(x)_m \\
&\quad \leqslant e^{-\beta U_1(x)_m} e^{(2\beta B+1)(m-1)} \sum_{n=0}^{\infty} |z|^n C(\beta)^n e^{n(2\beta B+1)} \\
&\quad \leqslant e^{-\beta U_1(x)_m} e^{(2\beta B+1)(m-1)} (1-|z|\, C(\beta)\, e^{2\beta B+1})^{-1} \qquad (2.20)
\end{aligned}$$

if $z \in D_\beta$. So the power series of $\rho_A(x)_m$ is absolutely convergent, hence $\rho_A(x)_m$ is an analytic function of z in D_β. Moreover, for all $m \geqslant 1$,

$$\rho(x)_m = z^m \sum_{n=0}^{\infty} \frac{z^n}{n!} \int d(y)_n \psi_{(x)_m}(y)_n \equiv z^m \psi^z(x)_m \qquad (2.21)$$

is also absolutely convergent and defines an analytic funtion of z in D_β. It is not difficult to see that $\rho = \lim_{A \to \mathbf{R}^D} \rho_A$. Indeed, if $(x)_m \subset A$,

$$\rho(x)_m - \rho_A(x)_m = z^m \sum_{n=1}^{\infty} \frac{z^n}{n!} \int_{(A^c)^n} d(y)_n \psi_{(x)_m}(y)_n \qquad (2.22)$$

The series is absolutely convergent,

$$|\rho(x)_m - \rho_A(x)_m| \leqslant |z|^m \sum_{n=1}^{\infty} \frac{|z|^n}{n!} \int_{(A^c)^n} d(y)_n |\psi_{(x)_m}(y)_n| \qquad (2.23)$$

On the right side of this inequality each term goes monotonically to zero with A going to $\mathbf{R}^D$ through an increasing sequence, so the sum goes to zero as well.

Each $\rho(x)_m$ is translation invariant; in particular, $\rho(x_1) \equiv \rho_1$, the density, which depends analytically on z in D_β. Translation invariance is inherited from the Boltzmann factors and Ursell functions via

$$\psi_{x_1+x,\dots,x_m+x}(y)_n = \psi_{(x)_m}(y)_n \qquad (2.24)$$

Now we turn to the proof of the bound (2.19). Denote

$$W_k((x)_m, (y)_n) = \sum_{i=1}^{m} \sum_{j=1}^{n} \phi_k(y_j - x_i), \qquad k = 1, 2$$
$$W = W_1 + W_2 \tag{2.25}$$

and

$$K(x, (y)_n) = \prod_{i=1}^{n} (e^{-\beta\phi(y_i - x)} - 1) \tag{2.26}$$

ψ satisfies the recurrence relation

$$\psi_X(Y) = e^{-\beta W(x_i, X_i)} \sum_{S \subset Y} K(x_i, S)\, \psi_{X_i \cup S}(Y \backslash S) \tag{2.27}$$

[cf. Eq. (4.26) in ref. 20]. Here $X = (x)_m$, $Y = (y)_n$, x_i is any element of X, and $X_i = X \backslash \{x_i\}$. Both S and $Y \backslash S$ are subsequences of Y. Notice that $\psi_{(x)_m}(y)_n$ is separately symmetric in the m, resp., n variables $(x)_m$ and $(y)_n$, therefore the notation $X_i \cup S$ is unambiguous. By integration over $(y)_n$, from Eq. (2.27) one obtains

$$\Psi_n(x)_m \leqslant e^{-\beta W(x_i, X_i)} \sum_{k=0}^{n} \frac{n!}{k!(n-k)!}$$
$$\times \int d(y)_k\, |K(x_i, (y)_k)|\, \Psi_{n-k}(X_i \cup (y)_k) \tag{2.28}$$

As in ref. 20, we proceed by induction on $m + n$. Let first $m = 1$, $n = 0$. Now, $\Psi_0(x_1) = (\psi_{x_1})_0 = \exp[-\beta U(x_1)] = 1$, so (2.19) holds for $m + n = 1$. Applying the induction hypothesis to the right side of the inequality (2.28), we get

$$\Psi_n(x)_m \leqslant n!\, C(\beta)^n e^{-\beta W(x_i, X_i)}\, e^{(2\beta B + 1)(m + n - 2)} \sum_{k=0}^{n} \frac{C(\beta)^{-k}}{k!}$$
$$\times \int |K(x_i, (y)_k)|\, e^{-\beta U_1(X_i \cup (y)_k)}\, d(y)_k$$
$$= n!\, C(\beta)^n\, e^{-\beta[U_1(x)_m + W_2(x_i, X_i)]}\, e^{(2\beta B + 1)(m + n - 2)} \sum_{k=0}^{n} \frac{I_k(x)_m}{k!\, C(\beta)^k} \tag{2.29}$$

where

$$I_k(x)_m = \int d(y)_k\, |K(x_i, (y)_k)|\, e^{-\beta[U_1(y)_k + W_1(X_i, (y)_k)]} \tag{2.30}$$

Notice that

$$U_2(x)_m = \tfrac{1}{2} \sum_{i=1}^{m} W_2(x_i, X_i) \geqslant -Bm \tag{2.31}$$

so $W_2(x_i, X_i) \geqslant -2B$ for suitably chosen i. Therefore Eq. (2.19) is verified, provided that

$$I_k(x)_m \leqslant C(\beta)^k \tag{2.32}$$

for all k, m, i and all admissible $(x)_m$. Now $I_k(x)_m$ can be written

$$\begin{aligned} I_k(x)_m = \int d(y)_k \prod_{j=1}^{k} \Bigg(&|\exp[-\beta\phi(y_j)] - 1| \\ &\times \exp\left\{-\beta\left[\sum_{l\neq i} \phi_1(y_j - x'_l) + \sum_{l=j+1}^{k} \phi_1(y_j - y_l)\right]\right\}\Bigg) \end{aligned} \tag{2.33}$$

where $x'_l = x_l - x_i$. If $U_1(x)_m < \infty$, then $U_1(X'_i) = U_1(X_i) < \infty$. On the other hand, the integrand vanishes if $U_1(y)_k = \infty$ or $W_1(X'_i, (y)_k) = \infty$, so that

$$\begin{aligned} I_k(x)_m = \int_{U_1(X'_i \cup (y)_k) < \infty} d(y)_k \prod_{j=1}^{k} \Bigg(&|\exp[-\beta\phi(y_j)] - 1| \\ &\times \exp\left\{-\beta\left[\sum_{l\neq i} \phi_1(y_j - x'_l) + \sum_{l=j+1}^{k} \phi_1(y_j - y_l)\right]\right\}\Bigg) \end{aligned} \tag{2.34}$$

which is clearly majorized by $C(\beta)^k$.

For $m = 1$ the bound (2.19) can be improved by a factor $e^{-2\beta B}$ because $U(x)_1 = 0$ and the first exponential factor on the right of Eq. (2.29) can be dropped. So we get

$$\Psi_n(x_1) \leqslant n!\, e^{-2\beta B} (C(\beta)\, e^{2\beta B + 1})^n \tag{2.35}$$

It remains to prove the cluster property (2.8). Here we fully rely upon ref. 20. The sequence $\rho = (\rho(x)_m)_{m \geqslant 0}$ of correlation functions ($\rho_0 = 1$) can be written $\rho \risingdotseq \operatorname{Exp} \rho^T$, where ρ^T is the sequence of truncated correlations. These are also invariant under translations. Therefore ρ^T depends only on the coordinate differences $x_j - x_i$. A sufficient condition to get (2.8) is that for any m and any $i \in \{2,..., m\}$, $\rho^T(x)_m \to 0$ with $|x_i - x_1| \to \infty$. This clearly holds if

$$\int dx_2 \cdots dx_m\, |\rho^T(x)_m| < \infty \tag{2.36}$$

To obtain an expression for ρ^T we return to Eq. (2.21). Since $\psi_0^z = 1$, introducing the cluster function ϕ^z of ψ^z, we have $\psi^z = \text{Exp}\,\phi^z$ and

$$\rho^T(x)_m = z^m \phi^z(x)_m \tag{2.37}$$

This ϕ^z is the same as Ruelle's. Referring to ref. 20 for the intermediate steps, one finally obtains, using the bound (2.35),

$$\begin{aligned}
&\int dx_2 \cdots dx_m \, |\phi^z(x)_m| \\
&\leqslant \sum_{n=0}^{\infty} \frac{|z|^n}{n!} \Psi_{n+m-1}(x_1) \\
&\leqslant (m-1)! \, e^{-2\beta B} \frac{(C(\beta)\, e^{2\beta B+1})^{m-1}}{(1-|z|\, C(\beta)\, e^{2\beta B+1})^m}
\end{aligned} \tag{2.38}$$

which is just Eq. (4.41) of ref. 20 with a different meaning of B and $C(\beta)$. This finishes the proof. ▮

2.3. Free Energy and Pressure at High Temperatures

We expect that under condition (C) the pressure

$$p_\Lambda = (\beta\, |\Lambda|)^{-1} \ln \Xi_\Lambda \tag{2.39}$$

and the free energy per particle

$$f_{\Lambda,N} = -(\beta N)^{-1} \ln Q_{\Lambda,N} \tag{2.40}$$

remain bounded as the volume $|\Lambda|$ tends to infinity, and the pressure depends analytically on z in the disk D_β. Both can be show under some additional hypotheses.

Theorem 2. (i) If $C(2\beta) < \infty$ and $z \in D_\beta$, the grand-canonical pressure $p_\Lambda(\beta, z)$ converges on Van Hove sequences and the limit is an analytic function of z in D_β.

(ii) If $C(\beta) < \infty$ holds with a ϕ_1 such that $\phi_1(x) \leqslant 0$ for $|x|$ sufficiently large, and $z \in D_\beta$, $p_\Lambda(\beta, z)$ converges on Van Hove sequences and the limit is an analytic function of z in D_β.

(iii) If $C(\beta) < \infty$ holds with $\phi = \phi_1$ and $\phi(x) < -\varepsilon < 0$ on some open set, then for any bounded Lebesgue-measurable Λ

$$\beta f_{\Lambda,N} \geqslant \ln(N/|\Lambda|) - 1 - \max\{1, \ln C(\beta)\, \rho_{\text{cp}}\} \tag{2.41}$$

and for any real, positive z

$$p_\Lambda(\beta, z) \leqslant z \max\{e, C(\beta)\, \rho_{\mathrm{cp}}\} \tag{2.42}$$

Here ρ_{cp} is the close-packing density.

Proof. (i)–(ii) The pressure p_Λ is related to the one-point distribution function through the equation

$$\beta p_\Lambda = |\Lambda|^{-1} \ln \Xi_\Lambda = \int_0^z \frac{dz}{z} |\Lambda|^{-1} \int dx_1\, \rho_\Lambda(x_1) \tag{2.43}$$

Suppose that

$$\lim_{|\Lambda| \to \infty} |\Lambda|^{-1} \int dx_1\, \rho_\Lambda(x_1) = \rho_1 \tag{2.44}$$

Then p_Λ converges to

$$p = \beta^{-1} \int_0^z \frac{dz}{z} \rho_1 \tag{2.45}$$

which depends analytically on z in D_β. We will prove Eq. (2.44) for Λ going to infinity in Van Hove sense.

Let $(x)_m \subset \Lambda$ and define

$$\Psi_n^\Lambda(x)_m = \int_{(\Lambda^c)^n} d(y)_n\, |\psi_{(x)_m}(y)_n| \tag{2.46}$$

This quantity satisfies the analog of the inequality (2.28) with the difference that all the integrals are restricted to Λ^c. The analog of (2.19) will also hold if $C(\beta)$ is replaced by some $C_{(x)_m}^\Lambda(\beta)$ chosen so that the analog of $I_n(x)_m$,

$$\begin{aligned} I_n^\Lambda(x)_m = \int_{(\Lambda^c)^n} & d(y)_n\, |K(x_m, (y)_n)| \\ & \times \exp[-\beta(U_1(y)_n + W_1((x)_{m-1}, (y)_n))] \\ & \leqslant C_{(x)_m}^\Lambda(\beta)^n \end{aligned} \tag{2.47}$$

for all $n \geqslant 0$ and all admissible $(x)_m \subset \Lambda$. A suitable choice is

$$\begin{aligned} C_{(x)_m}^\Lambda(\beta) = \max_i \sup_{Y \subset \Lambda^c:\, U_1(X_i, Y) < \infty} & \int_{\Lambda^c} dy\, |\exp[-\beta\phi(y - x_i)] - 1| \\ & \times \exp\left\{-\beta\left(\sum_{j \neq i} \phi_1(y - x_j) + \sum_{j=1}^n \phi_1(y - y_j)\right)\right\} \end{aligned} \tag{2.48}$$

where X_i, Y were introduced in Eq. (2.27). With this we get for $(x)_m \subset \Lambda$ [cf. Eq. (2.23)]

$$|\rho(x)_m - \rho_\Lambda(x)_m| \leqslant \sum_{n=1}^{\infty} \frac{|z|^{m+n}}{n!} \Psi_n^\Lambda(x)_m$$
$$\leqslant \frac{|z|^{m+1} C_{(x)_m}^\Lambda(\beta) \exp[-\beta U_1(x)_m + 2\beta B(m - \delta_{m,1}) + m]}{1 - |z| C_{(x)_m}^\Lambda(\beta) e^{2\beta B + 1}} \tag{2.49}$$

For $z \in D_\beta$ the upper bound is finite because $C_{(x)_m}^\Lambda(\beta) \leqslant C(\beta)$. The left member goes to zero with Λ increasing and tending to $\mathbf{R}^D$. This is not necessarily true for the upper bound, although

$$C_{(x)_m}^\Lambda \leqslant C_{(x)_m}^{\Lambda'} \qquad \text{for} \quad \Lambda \supset \Lambda'$$

is easily seen.

First we prove (i). Suppose $C(2\beta) < \infty$. Using the Schwarz inequality,

$$C_{(x)_m}^\Lambda(2\beta) \leqslant C(2\beta) \tag{2.50}$$

and

$$|e^{-\beta\phi(y - x_i)} - 1| \leqslant |e^{-2\beta\phi(y - x_i)} - 1| \tag{2.51}$$

we obtain

$$C_{(x)_m}^\Lambda(\beta) \leqslant \max_{1 \leqslant i \leqslant m} \left(C(2\beta) \int_{\Lambda^c} dy\, |\exp[-2\beta\phi(y - x_i)] - 1| \right.$$
$$\left. \times \exp\left[-2\beta \sum_{j \neq i} \phi_1(y - x_j) \right] \right)^{1/2} \tag{2.52}$$

which goes to zero if $\Lambda \to \mathbf{R}^D$. For $m = 1$ somewhat more holds true. In this case (2.52) reads

$$C_x^\Lambda(\beta) \leqslant \left[C(2\beta) \int_{\Lambda^c} |e^{-2\beta\phi(y - x)} - 1|\, dy \right]^{1/2} \tag{2.53}$$

Due to the invariance of ϕ under translations, the upper bound goes to zero if $\operatorname{dist}(x, \Lambda^c) \to \infty$. Thus, for any $\varepsilon > 0$ there is a finite r such that $C_x^\Lambda(\beta) < \varepsilon$ if $\operatorname{dist}(x, \Lambda^c) \geqslant r$. Let

$$\partial_r(\Lambda) = \{x \in \Lambda\colon \operatorname{dist}(x, \Lambda^c) \leqslant r\} \tag{2.54}$$

Then

$$|\Lambda|^{-1} \int_\Lambda |\rho_\Lambda(x) - \rho_1| \, dx \leqslant \frac{|z|^2 e}{1 - |z| \, C(\beta) \, e^{2\beta B + 1}} \left(\varepsilon + C(\beta) \frac{|\partial_r(\Lambda)|}{|\Lambda|} \right) \tag{2.55}$$

If Λ goes to infinity on a Van Hove sequence, $|\partial_r(\Lambda)|/|\Lambda| \to 0$ by definition and, ε being arbitrary, this proves the assertion.

Let us turn to the proof of (ii). Assume that $\phi_1(x) \leqslant 0$ if $|x| > R$ for some finite R. We show, as before, that $C_x^\Lambda \to 0$ if $\text{dist}(x, \Lambda^c) \to \infty$ (here and below we do not indicate the dependence on β, which is fixed). C_x^Λ is monotonically decreasing with increasing Λ; suppose it converges to some $C_x^\infty > 0$ as Λ increases to $\mathbf{R}^D$. Then there exists a bounded Λ_1 containing x and satisfying

$$C_x^{\Lambda_1} \leqslant (5/4) \, C_x^\infty$$

Also, one can find two bounded sets, $\Lambda_2 \subset \Lambda_3 \subset \mathbf{R}^D \equiv \Lambda_4$ with $\Lambda_1 \subset \Lambda_2$ and $\text{dist}(\Lambda_2, \Lambda_3^c) > R$, and coordinates $(y_1^i, ..., y_{n_i}^i) \subset \Lambda_{i+1} \backslash \Lambda_i$ with $U_1(y^i)_{n_i} < \infty$ $(i = 1, 3)$ such that

$$C_i = \int_{\Lambda_{i+1} \backslash \Lambda_i} dy \, |\exp[-\beta\phi(y-x)] - 1| \exp\left[-\beta \sum_{j=1}^{n_i} \phi_1(y - y_j^i) \right] > \tfrac{2}{3} C_x^\infty \tag{2.56}$$

for $i = 1, 3$. Now

$$\begin{aligned} \tfrac{5}{4} C_x^\infty \geqslant C_x^{\Lambda_1} &\geqslant \int_{\Lambda_1^c} dy \, |\exp[-\beta\phi(y-x)] - 1| \\ &\quad \times \exp\left[-\beta \left(\sum_{j=1}^{n_1} \phi_1(y - y_j^1) + \sum_{j=1}^{n_3} \phi_1(y - y_j^3) \right) \right] \\ &\geqslant C_1 + C_3 > \tfrac{4}{3} C_x^\infty \end{aligned} \tag{2.57}$$

From this contradiction we conclude that $C_x^\Lambda \to 0$ as $\text{dist}(x, \Lambda^c) \to \infty$. The proof can be completed as in case (i).

(iii) The proof consists of two steps. First, using that $C(\beta) < \infty$ holds with $\phi = \phi_1$, one shows that

$$Q_{\Lambda,n} \leqslant \frac{|\Lambda|}{n} \sum_{k=0}^{n-1} \frac{C(\beta)^k}{k!} Q_{\Lambda,n-k-1} \tag{2.58}$$

Second, from this inequality together with the fact that ϕ has a hard core (cf. Proposition 1) one deduces by induction that

$$Q_{\Lambda,n} \leqslant \frac{|\Lambda|^n}{n!} [\max\{e, C(\beta) \, \rho_{\text{cp}}\}]^n \tag{2.59}$$

Clearly, this implies the result on $f_{\Lambda,N}$ and p_Λ. The proof of (2.58) is analogous to that of Eq. (2.19):

$$\begin{aligned}
&\int_{\Lambda^n} d(y)_n\, e^{-\beta U(y)_n}\\
&\quad=\int_\Lambda dy_n \int_{\Lambda^{n-1}} d(y)_{n-1}\left(\prod_{i=1}^{n-1} e^{-\beta\phi(y_n-y_i)}\right) e^{-\beta U(y)_{n-1}}\\
&\quad=\int_\Lambda dy_n \sum_{Y\subset(y)_{n-1}} \int_{\Lambda^{|Y|}} dY\, K(y_n, Y)\int_{\Lambda^{n-1-|Y|}} d((y)_{n-1}\backslash Y)\, e^{-\beta U(y)_{n-1}}\\
&\quad=\int_\Lambda dy_n \sum_{k=0}^{n-1}\frac{(n-1)!}{k!\,(n-k-1)!}\int_{\Lambda^{n-k-1}} d(x)_{n-k-1}\, e^{-\beta U(x)_{n-k-1}}\\
&\qquad\times\int_{\Lambda^k} d(y)_k\, K(y_n,(y)_k)\, e^{-\beta(U(y)_k+W((x)_{n-k-1},(y)_k))}\\
&\quad\leqslant |\Lambda|\sum_{k=0}^{n-1}\frac{(n-1)!}{k!\,(n-k-1)!}\, C(\beta)^k\int_{\Lambda^{n-k-1}} d(x)_{n-k-1}\, e^{-\beta U(x)_{n-k-1}} \qquad (2.60)
\end{aligned}$$

In the inequality we used the bound (2.32), which holds because now $U=U_1$, $W=W_1$. Dividing by $n!$, we obtain (2.58). To prove (2.59) by induction, suppose that for $k\leqslant n-1$,

$$Q_{\Lambda,k}\leqslant (q\,|\Lambda|)^k/k! \qquad (2.61)$$

where

$$q=\max\{e,\, C(\beta)\,\rho_{\text{cp}}\} \qquad (2.62)$$

Now

$$Q_{\Lambda,n}\leqslant\frac{|\Lambda|}{n}\sum_{k=0}^{n-1}\frac{C(\beta)^k}{k!}\frac{(q\,|\Lambda|)^{n-k-1}}{(n-k-1)!}=\frac{|\Lambda|}{n!}\,(C(\beta)+q\,|\Lambda|)^{n-1}\leqslant\frac{(q\,|\Lambda|)^n}{n!} \qquad (2.63)$$

if

$$\left(1+\frac{C(\beta)}{q\,|\Lambda|}\right)^{n-1}\leqslant q \qquad (2.64)$$

Because of the hard core, it suffices to show (2.64) for $n\leqslant x_\Lambda=|\Lambda|\,\rho_{\text{cp}}$. Thus, we have to verify that

$$\left(1+\frac{C(\beta)\,\rho_{\text{cp}}}{qx_\Lambda}\right)^{x_\Lambda}\leqslant q \qquad (2.65)$$

However, $(1+x^{-1})^x < e$ for $x > 0$, so (2.65) holds if

$$e^{C(\beta)\rho_{cp}/q} \leqslant q \tag{2.66}$$

which is true for the choice (2.62). This closes the proof of the theorem. ∎

3. THE INTERACTIONS $\phi_{b,\alpha}$

Let us check condition (C) on the interactions $\phi_{b,\alpha}$; cf. Eq. (1.1). Choose $\phi_2 = 0$, so $\phi = \phi_1 = \phi_{b,\alpha}$. Let $(x)_m$ be any admissible set, i.e., $|x_i - x_j| \geqslant a$ for any $i \neq j$. Define

$$\begin{aligned}
A_0 &= \{ y \in \mathbf{R}^D \colon W(y, (x)_m) = 0 \} \\
B_0 &= \{ y \in \mathbf{R}^D \colon |y| < a \} \\
A_n &= \{ y \in \mathbf{R}^D \colon \max\{k \colon \, ||y - x_i| - b_k| < \alpha_k \text{ for some } i\} = n \}, \qquad n \geqslant 1 \\
B_n &= \{ y \in \mathbf{R}^D \colon ||y| - b_n| < \alpha_n \}, \qquad n \geqslant 1
\end{aligned} \tag{3.1}$$

Notice that $A_n = A_n(x)_m$ and B_n is independent of $(x)_m$. Then

$$\begin{aligned}
&\int dy \, |\exp[-\beta\phi(y)] - 1| \exp\left[-\beta \sum_{i=1}^{m} \phi(y - x_i) \right] \\
&\quad \leqslant \sum_{n=0}^{\infty} \exp\left[\beta \sum_{k=1}^{n} N_k(a) \, b_k^{-\mu} \right] \int_{A_n} dy \, |\exp[-\beta\phi(y)] - 1| \\
&\quad = \sum_{n=0}^{\infty} \exp\left[\beta \sum_{k=1}^{n} N_k(a) b_k^{-\mu} \right] \\
&\qquad \times \left(|A_n \cap B_0| + \sum_{l=1}^{\infty} [\exp(\beta b_l^{-\mu}) - 1] \, |A_n \cap B_l| \right)
\end{aligned} \tag{3.2}$$

where $|X|$ denotes the Lebesgue measure of $X \subset \mathbf{R}^D$. Here $N_k(a)$ is the maximum number of hard balls of diameter a which can be placed with the centers in a spherical layer of central radius b_k and width $2\alpha_k$. It is proportional to the surface area of a sphere of radius b_k, so there is some $c_1 > 0$ such that

$$N_k(a) \leqslant c_1 b_k^{D-1} \tag{3.3}$$

In one dimension we have equality with $c_1 = 2$.

We also need an upper bound to $|A_n \cap B_l|$, independent of $(x)_m$. Such a bound exists because of the condition $|x_i - x_j| \geqslant a$ for $i \neq j$. First, there is a $c_2 > 0$ such that

$$|A_0 \cap B_l| \leqslant |B_l| \leqslant c_2 \alpha_l b_l^{D-1} \qquad \text{for} \quad l \geqslant 1 \tag{3.4}$$

Second, there is a $c_3 > 0$ such that for any $n \geqslant 1$

$$|A_n \cap B_0| \leqslant c_3 \alpha_n b_n^{D-1} \tag{3.5}$$

This bound is obtained by observing that for

$$b_n - 2a - \alpha_n < \operatorname{dist}(x_i, B_0) < b_n + \alpha_n \tag{3.6}$$

one has

$$|\{y \in B_0: ||y - x_i| - b_n| < \alpha_n\}| \leqslant c_3' \alpha_n \tag{3.7}$$

and the maximum number of hard spheres at a suitable distance (3.6) from B_0 is less than $c_3'' b_n^{D-1}$. Third, there is a $c_4 > 0$ such that for any $n \geqslant 1$, $l \geqslant 1$,

$$|A_n \cap B_l| \leqslant \min\{c_2 \alpha_l b_l^{D-1}, c_4 \alpha_n b_l^D (b_l + b_n)^{D-1}\} \tag{3.8}$$

The first member on the right is the upper bound (3.4) to $|B_l|$. The second is the product of

$$|\{y \in B_l: ||y - x_i| - b_n| < \alpha_n\}| \leqslant c_4' \alpha_n b_l^{D-1} \tag{3.9}$$

(here i is fixed) with the largest number of hard balls at a suitable distance from B_l, which is bounded by some multiple of $b_l(b_l + b_n)^{D-1}$. Substituting Eqs. (3.3)–(3.5) and (3.8) into Eq. (3.2) and taking the supremum over $(x)_m$,

$$\begin{aligned} C(\beta) \leqslant c_0 + c_2 \sum_{l=1}^{\infty} [\exp(\beta b_l^{-\mu}) - 1]\, \alpha_l b_l^{D-1} \\ + \sum_{n=1}^{\infty} \left[\exp\left(\beta c_1 \sum_{k=1}^{n} b_k^{D-1-\mu} \right) \right] \\ \times \left\{ c_3 \alpha_n b_n^{D-1} + c_5 \alpha_n b_n^{D-1} \sum_{l=1}^{n} [\exp(\beta b_l^{-\mu}) - 1]\, b_l^D \right. \\ \left. + c_2 \sum_{l=n+1}^{\infty} [\exp(\beta b_l^{-\mu} - 1]\, \alpha_l b_l^{D-1} \right\} \end{aligned} \tag{3.10}$$

where $c_0 = |B_0|$ and $c_5 = 2^{D-1} c_4$.

It is obvious that for any positive sequence b_n tending monotonically to infinity one can choose α_n sufficiently rapidly decaying so that the upper bound is convergent for all $\beta < \infty$, hence $C(\beta) < \infty$ for all $\beta < \infty$. Some of these interactions are manifestly unstable. For instance, $b_n = n$ and $\mu \leqslant 1$ defines an unstable interaction in any dimension, as it is seen from Eq. (1.3). Thus, we have examples of unstable interactions which do not lead to a catastrophe at low temperatures.

For $D = 1$ and $b_n = n$ we can replace Eq. (3.8) by the stronger

$$|A_n \cap B_l| \leqslant \min\{4\alpha_l, 8\alpha_n\} \tag{3.11}$$

With this the inequality (3.10) reads

$$\begin{aligned} C(\beta) \leqslant c_0 + c_2 \sum_{l=1}^{\infty} [\exp(\beta l^{-\mu}) - 1]\, \alpha_l + \sum_{n=1}^{\infty} \left[\exp\left(2\beta \sum_{k=1}^{n} k^{-\mu} \right) \right] \\ \times \left\{ c_3 \alpha_n + 8\alpha_n \sum_{l=1}^{n} [\exp(\beta l^{-\mu}) - 1] + 4 \sum_{l=n+1}^{\infty} [\exp(\beta l^{-\mu}) - 1]\, \alpha_l \right\} \end{aligned} \tag{3.12}$$

If $\mu = 1$, there is a $K > 0$ such that

$$C(\beta) \leqslant K \left(\sum_{l=1}^{\infty} \alpha_l l^{-1} + \sum_{n=1}^{\infty} n^{2\beta} \left(\alpha_n \ln n + \sum_{l=n+1}^{\infty} \alpha_l l^{-1} \right) \right) \tag{3.13}$$

Let $\alpha_n = cn^{-\nu}$ with $\nu > 1$, as in Eq. (1.2). The first sum is convergent; therefore $C(\beta) < \infty$ if

$$\sum_{n=1}^{\infty} n^{2\beta - \nu} \ln n < \infty \tag{3.14}$$

and this holds for $\beta < \frac{1}{2}(\nu - 1)$. If $\alpha_n = o(n^{-\nu})$ for any $\nu > 1$, then $C(\beta) < \infty$ for all $\beta < \infty$.

If $0 \leqslant \mu < 1$, there is some $K > 0$ such that

$$C(\beta) \leqslant K \left(\sum_{l=1}^{\infty} \alpha_l + \sum_{n=1}^{\infty} e^{[2\beta/(1-\mu)] n^{1-\mu}} \left(\alpha_n n + \sum_{l=n+1}^{\infty} \alpha_l \right) \right) \tag{3.15}$$

Let $\alpha_n = c^{n^{1-\mu}}$ (with $c < 1$) as in Eq. (1.2). The first sum is convergent; therefore $C(\beta) < \infty$ if

$$\sum_{n=1}^{\infty} n \exp\left[\left(\frac{2\beta}{1-\mu} + \ln c \right) n^{1-\mu} \right] < \infty \tag{3.16}$$

which holds for $\beta < \frac{1}{2}(1-\mu) \ln c^{-1}$.

Finally, let $\mu<0$. There is a $K>0$ such that

$$C(\beta)\leqslant K\left(\sum_{l=1}^{\infty} e^{\beta l^{-\mu}}\alpha_l+\sum_{n=1}^{\infty} e^{[2\beta/(1-\mu)]n^{1-\mu}}\left(\alpha_n n e^{\beta n^{-\mu}}+\sum_{l=n+1}^{\infty} e^{\beta l^{-\mu}}\alpha_l\right)\right) \tag{3.17}$$

Choose $\alpha_n=c^{n^{1-\mu}}$, $c<1$. The first sum is convergent for all β, so $C(\beta)<\infty$ if

$$\sum_{n=1}^{\infty}\left\{\exp\left[\left(\frac{2\beta}{1-\mu}+\ln c\right)n^{1-\mu}\right]\right\}n\exp(\beta n^{-\mu})<\infty \tag{3.18}$$

which, again, holds for $\beta<\frac{1}{2}(1-\mu)\ln c^{-1}$. For every $\mu<1$, $\alpha_n=r^{n^{\nu}}$ with $r<1$ and $\nu>1-\mu$ implies $C(\beta)<\infty$ for all $\beta<\infty$.

4. A MODEL OF CRYSTALLIZATION

4.1. Ground States

We are interested in the ground states of a system of N particles on a one-dimensional interval Λ of length L interacting via the pair interaction φ defined in the Introduction. We confine ourselves to a qualitative discussion.

To describe the ground states it is useful to introduce the following notation: Given the sequences b_k and α_k as specified after Eq. (1.1), for a distance r,

$$r\approx b_k \qquad \text{if} \quad b_k-\alpha_k<r<b_k+\alpha_k \tag{4.1}$$

In particular, if $b_k=k$, we say that r is an approximate integer if the above holds.

A configuration $(x)_N$ with every x_i in Λ is an N-particle ground state if

$$U(x)_N=\min_{y_i\in\Lambda} U(y)_N$$

The easiest case is $0<\mu\leqslant 1$. If $\rho=N/L\leqslant 1$, the ground states of φ are the configurations

$$x_1<\cdots<x_N, \qquad x_j-x_i\approx j-i \qquad (j>i) \tag{4.2}$$

and their permutations. They are independent of the density and can be called single or pure crystals of period (density) 1. The formula (1.3) gives the energy of such configurations. If $\rho > 1$, no ground state can be a pure crystal. If $\rho \leqslant \lfloor a^{-1} \rfloor$, any ground state is formed by $\lceil \rho \rceil$ intercalated pure crystals of period 1 ($\lfloor \cdot \rfloor$ and $\lceil \cdot \rceil$ mean rounding downward and upward, respectively). If a^{-1} is not an integer, for $\rho \in (\lfloor a^{-1} \rfloor, a^{-1})$ there may be a competition among different "phase-separated" configurations. To minimize the energy, one or more chains of particles at approximate integer distances have to be present, mixed up with a disordered (fluid) component of density larger than ρ. The order within the chains may depend sensitively on the Diophantine properties of ρ, and we do not attempt any detailed discussion here.

If $\mu = 0$, any $(x)_N$ with $|x_j - x_i| \approx$ integer for each pair i, j is a ground state. The energy is still given by Eq. (1.3), that is, $E_\mu(N) = -N(N-1)/2$.

The case $\mu < 0$ is qualitatively different. Consider only $\rho \leqslant 1$. The interaction is actually repulsive; the particles tend to increase their mutual distances. As a result, in ground states

$$\max x_i - \min x_i \approx \lfloor L \rfloor$$

and the other positions depend on the density. In finite volumes it is difficult to give them precisely. It surely holds that $|x_j - x_i| \approx$ integer. Fixing one coordinate to be 0 and letting Λ tend to $\mathbf{R}$, $N \to \infty$ with $N/L = \rho$, one may ask what can be a limit of finite-volume ground states. The *presumably* correct answer is that for $\rho = p/q$, where p and q are relatively primes, one obtains a periodic subset of $\mathbf{Z}$ of period length q, while for irrational ρ the result is some quasiperiodic subset of $\mathbf{Z}$. For $\mu < 0$ the formula (1.3) gives an upper bound to the ground-state energy.

4.2. A Nonrigorous Energy-Entropy Argument

Let us choose $\rho \leqslant 1$ and compare the free energy of two restricted (microcanonical) ensembles of given energy: The first is the set of configurations (4.2), characteristic of a crystal, the second is the set of configurations of "free" particles $[U(x)_N = 0]$, characteristic of the fluid phase.

The energy in the first ensemble is given by Eq. (1.3). The volume in configuration space associated with (4.2) is bounded below by α_N^N and above by

$$L(2\alpha_1) \cdots (2\alpha_{N-1})$$

Therefore, the specific free energy of the first restricted ensemble is asymptotically

$$f_1(\mu) \asymp \begin{cases} (\beta^{-1}\nu - 1)\ln N & \text{if } \mu = 1 \\ \left(\beta^{-1}\zeta(N)\ln c^{-1} - \dfrac{1}{(1-\mu)(2-\mu)}\right) N^{1-\mu} & \text{if } \mu < 1 \end{cases} \tag{4.3}$$

with $(2-\mu)^{-1} \leqslant \zeta(N) \leqslant 1$.

Particle coordinates $x_1 < \cdots < x_N$ yielding $U(x)_N = 0$ occupy in Λ^N a volume of the order of $(c_0 N)^N/N!$, where c_0 is some bounded function of N. [Indeed, this volume can be estimated by neglecting the intervals of lengths $2\alpha_n$; then we get the partition function of a system of hard rods of length a (Tonks gas,[21]) which is of the proposed form with $c_0 = \rho^{-1} - a + a/N$. The actual c_0 is somewhat smaller.] Therefore the specific free energy of the second restricted ensemble is $f_2 = O(1)$ for all β. At high temperatures, $f_2 < f_1$, implying that the system is in a fluid phase. At $\beta > \beta_t$, where

$$\beta_t = \begin{cases} \nu & \text{if } \mu = 1 \\ (1-\mu)(2-\mu)\ln c^{-1} & \text{if } \mu < 1 \end{cases} \tag{4.4}$$

f_1 becomes smaller than f_2, indicating a transition to the solid phase.

4.3. Divergence of Thermodynamic Quantities

Let Λ denote the interval $[0, L]$. Recall that a is the length of the hard rods, so a^{-1} is the close packing density.

Proposition 2. For any $\rho < a^{-1}$ and any $\beta > \beta_t$, the free energy per particle $f_{\Lambda,N} \to -\infty$ as $N, L \to \infty$, $N/L = \rho$.

Proof. First, let $\rho < 1$. The right side of Eq. (4.3) [with $\zeta(N) = 1$] is the asymptotically leading order of a rigorous upper bound to $f_{\Lambda,N}$, and this implies the result.

If $1 \leqslant \rho < a^{-1}$, one can proceed as follows. Choose $\varepsilon > 0$ such that $\rho(a+\varepsilon) < 1$. Let

$$K = \left\lfloor L \frac{1 - \rho(a+\varepsilon)}{1 - a - \varepsilon} \right\rfloor \tag{4.5}$$

A lower bound to the partition function $Q_{\Lambda,N}$ can be obtained by allowing

$$x_i \in [i, i + \alpha_K), \qquad i = 1, 2, \ldots, K$$

and placing $x_{K+1},..., x_N$ between $K+\alpha_K$ and L. For these configurations $U(x)_N \leqslant E_\mu(K)$ and the occupied volume in the configuration space is $\geqslant \alpha_K^K(\varepsilon-\eta_L)^{N-K}$, where $\eta_L = O(L^{-1})$. This yields

$$Q_{\Lambda,N} \geqslant \alpha_K^K e^{-\beta E_\mu(K)}(\varepsilon-\eta_L)^{N-K} \tag{4.6}$$

and

$$f_{\Lambda,N} \leqslant (1-\beta_t/\beta)\, E_\mu(K)/K + O(1) \tag{4.7}$$

Because of $K = O(N)$, the result follows again. ∎

From the above proposition we immediately get the following result.

Corollary. For $\beta > \beta_t$ and any $z > 0$, the grand-canonical pressure $p_\Lambda \to \infty$ as $L \to \infty$.

As will be seen later, the limiting state of the canonical ensemble is highly singular, namely, the correlation functions exist only in distribution sense. Under such circumstances one cannot expect equivalence of the canonical and grand-canonical ensembles. For example, we do not expect that the canonical pressure

$$p_{\Lambda,N} = (\beta Q_{\Lambda,N})^{-1} \frac{\partial Q_{\Lambda,N}}{\partial L} = -\frac{\partial f_{\Lambda,N}}{\partial \rho^{-1}} \tag{4.8}$$

diverges for $\mu > 0$ and $\rho < 1$ as $N, L \to \infty$, $N/L = \rho$. However, for $\mu < 0$ and also for $\mu > 0$ and $\rho \geqslant 1$, $p_{\Lambda,N}$ may well tend to infinity with the increasing volume. This can be better seen from the following formula for $p_{\Lambda,N}$. Employing a rigid-wall boundary condition and using the translation and permutation invariance of $U(x_1,..., x_N)$, we find

$$\frac{\partial Q_{\Lambda,N}}{\partial L} = \frac{1}{(N-1)!} \int_0^L dx_1 \cdots \int_0^L dx_{N-1}\, e^{-\beta U(x_1,...,x_{N-1},L)} = Q_{\Lambda,N}\rho_{\Lambda,N}(L) \tag{4.9}$$

Here $\rho_{\Lambda,N}(x)$ is the one-point correlation (distribution) function in the canonical description, which can be interpreted as the (unnormalized) probability density for any particle to have position x, irrespective of the positions of the remaining particles. Because of

$$U(L-x_1,..., L-x_N) = U(x_1,..., x_N) \tag{4.10}$$

$\rho_{\Lambda,N}(L) = \rho_{\Lambda,N}(0)$, and the pressure can be written as

$$p_{\Lambda,N} = \beta^{-1}\rho_{\Lambda,N}(0) = \beta^{-1}\rho_{\Lambda,N}(L) = \tfrac{1}{2}\beta^{-1}[\rho_{\Lambda,N}(0) + \rho_{\Lambda,N}(L)] \tag{4.11}$$

This expression is generally valid in one dimension, under the symmetry conditions on $U(x)_N$. To get (4.9), we suppose also that the discontinuities of the n-particle interactions (which depend on $n-1$ distances) are in a set of zero Lebesgue measure in $\mathbf{R}^{n-1}$. If there is no interaction, $\rho_{\Lambda,N}(x)=\rho$ independent of x, and one obtains the ideal gas law. In the actual model if, e.g., $L\to\infty$ through integer values and $N>L$ or if $\mu<0$, the effective repulsion among the particles can make $\rho_{\Lambda,N}(x)$ tend to ∞ at $x=0$, L, implying the divergence of $p_{\Lambda,N}$.

4.4. Nondecaying Pair Correlations

Below we show the existence of nondecaying pair correlations at $\beta>\beta_t$. We work in the canonical ensemble, use a rigid-wall boundary condition, and, for convenience, restrict the discussion to densities $\rho\leqslant 1$.

The probability of an event A with support in Λ^N is

$$P_{\Lambda,N}(A)=\int_A e^{-\beta U(x)_N}\,d(x)_N\Big/\int_{\Lambda^N} e^{-\beta U(x)_N}\,d(x)_N \tag{4.12}$$

Because $U(x)_N$ is a symmetric function of $x_1,\ldots,x_N$, $P_{\Lambda,N}$ is invariant under permutations: Let π be any permutation of $\{1,\ldots,N\}$ and

$$\pi A=\{(x_{\pi(1)},\ldots,x_{\pi(N)}):(x)_N\in A\} \tag{4.13}$$

Then

$$P_{\Lambda,N}(\pi A)=P_{\Lambda,N}(A) \tag{4.14}$$

For any real x and $K>0$ define

$$\begin{aligned} S_K(x)&=\bigcup_{k\in\mathbf{Z},k>K}\{y\in\mathbf{R}: |y-x|\approx k\}\\ &=\bigcup_{k\in\mathbf{Z},|k|>K}(x+k-\alpha_{|k|},x+k+\alpha_{|k|}) \end{aligned} \tag{4.15}$$

Notice that $\operatorname{dist}(x,S_K(x))>K-1$. Furthermore, the Lebesgue measure of $S_K(x)$,

$$|S_K(x)|=4\sum_{k>K}\alpha_k \tag{4.16}$$

is independent of x, and goes to zero with K going to infinity, because $\sum\alpha_k$ is convergent.

Recall the definition of the pair correlation function in the canonical ensemble:

$$\rho_{\Lambda,N}(x_1, x_2) = N(N-1)\,\chi_\Lambda(x_1)\,\chi_\Lambda(x_2)\,\frac{\int_{\Lambda^{N-2}} e^{-\beta U(x)_N}\,dx_3 \cdots dx_N}{\int_{\Lambda^N} e^{-\beta U(x)_N}\,d(x)_N} \tag{4.17}$$

[cf. Eq. (2.1)]. $\rho_{\Lambda,N}(x_1, x_2)$ is the (unnormalized) probability density for any two particles to have positions x_1, x_2 irrespective of the positions of the remaining particles.

Below, $\#A$ denotes the number of points in the finite set A.

Theorem 3. Let Λ be an interval of length L, $\rho = N/L \leqslant 1$, and $\beta > \beta_t$. There exists a $\delta > 0$ and a function $K(N)$, $K(N) \to \infty$ as $N \to \infty$, such that for N sufficiently large

$$\max_{x_1}\ \max_{x_2 \in S_{K(N)}(x_1)} \rho_{\Lambda,N}(x_1, x_2) \geqslant \delta\rho/|S_{K(N)}| \tag{4.18}$$

Furthermore, for any i,

$$P_{\Lambda,N}(\#\{j: |x_j - x_i| \approx \text{integer}\} > K(N)) \geqslant \delta \tag{4.19}$$

This theorem shows the existence of long-range correlations. As $L, N \to \infty$, $\operatorname{dist}(x, S_{K(N)}(x)) \to \infty$ and $|S_{K(N)}| \to 0$; thus the pair correlation function develops increasing maxima at longer and longer integer distances. In the absence of ordering $\rho_{\Lambda,N}(x_1, x_2)$ would asymptotically factorize to $\rho_{\Lambda,N}(x_1)\,\rho_{\Lambda,N}(x_2)$ as $|x_2 - x_1|$ tends to infinity, and none of the factors would diverge: so $\rho_{\Lambda,N}(x_1, x_2)$ would remain uniformly bounded.

The theorem remains valid for periodic boundary condition (with suitable modification of the interaction); in this case the maximum over x_1 can be dropped.

Proof. Suppose we can prove that

$$P_{\Lambda,N}(\{x_i\}_{i=2}^N \cap S_{K(N)}(x_1) \neq \varnothing) \geqslant \delta \tag{4.20}$$

Then

$$\begin{aligned}
\delta &\leqslant P_{\Lambda,N}(\{x_i\}_{i=2}^N \cap S_{K(N)}(x_1) \neq \varnothing) \\
&= P_{\Lambda,N}\left(\bigcup_{i=2}^N \{x_i \in S_{K(N)}(x_1)\}\right) \\
&\leqslant \sum_{i=2}^N P_{\Lambda,N}(x_i \in S_{K(N)}(x_1)) \\
&= (N-1)\,P_{\Lambda,N}(x_2 \in S_{K(N)}(x_1))
\end{aligned}$$

$$= (N-1)\frac{\int_\Lambda dx_1 \int_{S_{K(N)}(x_1)} dx_2 \int_\Lambda dx_3 \cdots \int_\Lambda dx_N \exp - \beta U(x)_N}{\int_\Lambda dx_1 \cdots \int_\Lambda dx_N \exp - \beta U(x)_N}$$

$$= \frac{1}{N} \int_\Lambda dx_1 \int_{S_{K(N)}(x_1)} dx_2\, \rho_{\Lambda,N}(x_1, x_2)$$

$$\leqslant \frac{|S_{K(N)}|}{\rho} \max_{x_1} \max_{x_2 \in S_{K(N)}(x_1)} \rho_{\Lambda,N}(x_1, x_2) \tag{4.21}$$

which is just what was claimed.

To prove Eqs. (4.20) and (4.19), we need four lemmas.

Lemma 1. Let $\kappa < 1 - \beta_t/\beta$. Then

$$P_{\Lambda,N}(U(x)_N < \kappa E_\mu(N)) \geqslant 1 - \varepsilon_N \tag{4.22}$$

where ε_N goes to 0 as N increases.

Proof. We have

$$P_{\Lambda,N}(U(x)_N \geqslant \kappa E_\mu(N)) \leqslant \frac{(L^N/N!)\, e^{-\beta\kappa E_\mu(N)}}{\alpha_N^N e^{-\beta E_\mu(N)}} < e^{\beta(1-\kappa)E_\mu(N)} \left(\frac{e}{\rho\alpha_N}\right)^N \tag{4.23}$$

To get the first inequality, in the denominator we retained only the configurations (4.2). For the second inequality we used Stirling's formula $[N! > (N/e)^N]$. From (4.23) the result follows via Eqs. (1.2), (1.3) and (4.4), with an ε_N going to zero faster than any exponential $[\log \varepsilon_N = O(E_\mu(N))]$. ∎

Let $e_\mu(N) = |E_\mu(N)|/N$ and

$$w_i(x)_N = -\sum_{j \neq i} \varphi(x_j - x_i) \tag{4.24}$$

which is minus the potential energy of the ith particle in the configuration $(x)_N$. For any real η let

$$M_\eta(x)_N = \#\{i : w_i(x)_N > \eta e_\mu(N)\} \tag{4.25}$$

If $\eta < 2$ and N is large enough, this number may not be zero. To see this, notice first that Eq. (1.3) implies

$$e_\mu(N) \asymp \begin{cases} \ln N & \text{if } \mu = 1 \\ \dfrac{N^{1-\mu}}{(1-\mu)(2-\mu)} & \text{if } \mu < 1 \end{cases} \tag{4.26}$$

On the other hand, for $\mu \geqslant 0$

$$w_i(x)_N \leqslant 2 \sum_{n=1}^{N/2} n^{-\mu} \asymp \begin{cases} 2 \ln N & \text{if} \quad \mu = 1 \\ \dfrac{2^\mu}{1-\mu} N^{1-\mu} & \text{if} \quad \mu < 1 \end{cases} \tag{4.27}$$

and the inequality saturates (for the particles in the middle) in ground states. Comparing Eqs. (4.26) and (4.27), we see that

$$\max w_i(x)_N \asymp 2e_\mu(N) \qquad \text{if} \quad \mu = 0, 1 \tag{4.28}$$

and

$$\max w_i(x)_N > 2e_\mu(N) \qquad \text{if} \quad 0 < \mu < 1 \tag{4.29}$$

(because $2-\mu \geqslant 2^{1-\mu}$ in this interval).

If $\mu < 0$,

$$w_i(x)_N \leqslant \sum_{L-N \leqslant n \leqslant L} n^{-\mu} \asymp \frac{L^{1-\mu} - (L-N)^{1-\mu}}{1-\mu} \leqslant \frac{\rho^{-1+\mu}}{1-\mu} N^{1-\mu} \tag{4.30}$$

and in any ground state $(x^0)_N$, for the particles on the ends of the chain

$$w_i(x^0)_N \geqslant \sum_{n=1}^{N} n^{-\mu} \asymp (2-\mu)\, e_\mu(N) > 2e_\mu(N) \tag{4.31}$$

Lemma 2. Let $\kappa < 1$ and $\eta < 2\kappa$. For N sufficiently large,

$$U(x)_N < \kappa E_\mu(N) \qquad \text{implies} \quad M_\eta(x)_N > \frac{2\kappa - \eta}{g_\mu - \eta} N$$

were

$$g_\mu = \begin{cases} 3 & \text{if} \quad \mu = 1 \\ 2(2-\mu) & \text{if} \quad 0 \leqslant \mu < 1 \\ \rho^{-1+\mu}(2-\mu) & \text{if} \quad \mu < 0 \end{cases} \tag{4.32}$$

Proof. Comparing Eq. (4.26) with Eqs. (4.27) and (4.30), we find that for every $\mu \leqslant 1$ and N large enough,

$$w_i(x)_N \leqslant g_\mu e_\mu(N) \tag{4.33}$$

uniformly in $(x)_N$. Therefore

$$2\kappa\, |E_\mu(N)| < 2\, |U(x)_N| = \sum_{i=1}^{N} w_i(x)_N \leqslant (N - M_\eta(x)_N)\, \eta e_\mu(N) + g_\mu M_\eta(x)_N\, e_\mu(N) \tag{4.34}$$

or

$$2\kappa N < N\eta + (g_\mu - \eta)\, M_\eta(x)_N \tag{4.35}$$

which proves the assertion. ▌

From the above two lemmas one obtains

$$P_{\Lambda,N}\left(M_\eta(x)_N > \frac{2\kappa - \eta}{g_\mu - \eta} N\right) \geqslant P_{\Lambda,N}(U(x)_N < \kappa E_\mu(N)) \geqslant 1 - \varepsilon_N \tag{4.36}$$

if $\kappa < 1 - \beta_t/\beta$ and $\eta < 2\kappa$.

The proof of the following lemma is left to the reader.

Lemma 3. Let $\xi_1, ..., \xi_N$ be random variables from a probability space $(\Omega, \mathscr{F}, P)$ to a measurable space $(\Omega', \mathscr{F}')$ such that their joint probability distribution is permutation invariant. Then for any $A \in \mathscr{F}'$ and any i

$$P(\xi_i \in A \mid \#\{j\colon \xi_j \in A\} = k) = k/N \tag{4.37}$$

and

$$P(\xi_i \in A \mid \#\{j\colon \xi_j \in A\} \geqslant k\} \geqslant k/N \tag{4.38}$$

From the last inequality one finds for any i

$$P(\xi_i \in A) \geqslant \frac{k}{N} P(\#\{j\colon \xi_j \in A\} \geqslant k) \tag{4.39}$$

In the present problem, the event $\xi_i \in A$ corresponds to $w_i(x)_N > \eta e_\mu(N)$ and we get for any i

$$P_{\Lambda,N}(w_i(x)_N > \eta e_\mu(N)) \geqslant \frac{2\kappa - \eta}{g_\mu - \eta} P_{\Lambda,N}\left(M_\eta(x)_N > \frac{2\kappa - \eta}{g_\mu - \eta} N\right) \geqslant \frac{2\kappa - \eta}{g_\mu - \eta}(1 - \varepsilon_N) \tag{4.40}$$

which holds for any $\kappa < 1 - \beta_t/\beta$ and $\eta < 2\kappa$.

Lemma 4. For $\eta < 2$ and N sufficiently large, $w_i(x)_N > \eta e_\mu(N)$ implies

$$\{x_j\}_{j \neq i} \cap S_{K(N)}(x_i) \neq \varnothing \qquad \text{and} \qquad \#\{\, j\colon |x_j - x_i| \approx \text{integer}\} > K(N)$$

where

$$K(N) = \begin{cases} \dfrac{1}{2} N^{\eta/2} & \text{if } \mu = 1 \\ \dfrac{1}{2} \left(\dfrac{2^{-\mu}\eta}{2-\mu} \right)^{1/(1-\mu)} N & \text{if } 0 \leqslant \mu < 1 \\ \dfrac{1}{2} \left(\dfrac{1}{\rho} - \left(\dfrac{1}{\rho^{1-\mu}} - \dfrac{\eta}{2-\mu} \right)^{1/(1-\mu)} \right) N & \text{if } \mu < 0 \end{cases} \tag{4.41}$$

Proof. We have

$$w_i(x)_N = \sum_{n \geqslant 1} \#\{j\colon |x_j - x_i| \approx n\}\; n^{-\mu} \tag{4.42}$$

Let $k = \#\{j\colon |x_j - x_i| \approx \text{integer}\}$. Then

$$\eta e_\mu(N) < w_i(x)_N \leqslant \begin{cases} 2 \displaystyle\sum_{1 \leqslant n \leqslant k/2} n^{-\mu} & \text{if } 0 \leqslant \mu \leqslant 1 \\ \displaystyle\sum_{L-k \leqslant n \leqslant L} n^{-\mu} & \text{if } \mu < 0 \end{cases} \tag{4.43}$$

Comparing the asymptotic forms (4.26), (4.27), and (4.30) of the left and right ends of the above inequalities, we obtain that either $k > 2K(N)$ or $k \asymp 2K(N)$, so in both cases $k > K(N)$ for N large. This implies that the largest approximate integer distance between x_i and one of x_j, $j \neq i$, exceeds $K(N)$, as claimed. ▮

To finish the proof, choose $\eta < 2(1 - \beta_t/\beta)$ first; this determines $K(N)$ through Eq. (4.41). Let then

$$2\kappa = 1 - \beta_t/\beta + \eta/2 \tag{4.44}$$

which satisfies the inequalities $\eta < 2\kappa < 2(1 - \beta_t/\beta)$. Finally, choose N so large that the above lemmas hold and $\varepsilon_N < 1/2$. Then

$$\begin{aligned} P_{\Lambda,N}(\{x_i\}_{i=2}^{N} \cap S_{K(N)}(x_1) \neq \varnothing) &\geqslant P_{\Lambda,N}(w_1(x)_N > \eta e_\mu(N)) \\ &\geqslant \frac{1 - \beta_t/\beta - \eta/2}{2(g_\mu - \eta)} \equiv \delta \end{aligned} \tag{4.45}$$

The first inequality follows from the last lemma, the second is the same as (4.40). As a result, we obtained (4.20). The left member of the first inequality can be replaced by the left member of (4.19), which proves the second half of the theorem. ▌

Let us summarize what we have obtained for the one-dimensional model of crystallization.

Proposition 3. The one-dimensional interaction defined through Eqs. (1.1) and (1.2) satisfies condition (C) for $\mu = 1$ if $\beta < \frac{1}{2}(\nu - 1)$ and for $\mu < 1$ if $\beta < \frac{1}{2}(1-\mu)\ln c^{-1}$. In this temperature range the free energy per particle and the pressure remain finite in the thermodynamic limit, the pressure depends analytically on z in D_β, and the results of Theorem 1 on the correlation functions are valid.

Together with Proposition 2 and Theorem 3, this result implies that there occurs at least one phase transition at some β in the interval

$$\tfrac{1}{2}(\nu - 1) \leqslant \beta \leqslant \nu \qquad \text{if} \quad \mu = 1$$

and

$$\tfrac{1}{2}(1-\mu)\ln c^{-1} \leqslant \beta \leqslant (1-\mu)(2-\mu)\ln c^{-1} \qquad \text{if} \quad \mu < 1$$

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