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Wall-Induced Density Profiles and Density Correlations in Confined Takahashi Lattice Gases

J. Buschle,[1] P. Maass,[1] and W. Dieterich[1]

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We propose a general formalism to study the static properties of a system composed of particles with nearest neighbor interactions that are located on the sites of a one-dimensional lattice confined by walls ("confined Takahashi lattice gas"). Linear recursion relations for generalized partition functions are derived, from which thermodynamic quantities, as well as density distributions and correlation functions of arbitrary order can be determined in the presence of an external potential. Explicit results for density profiles and pair correlations near a wall are presented for various situations. As a special case of the Takahashi model we consider in particular the hard rod lattice gas, for which a system of nonlinear coupled difference equations for the occupation probabilities has been presented by Robledo and Varea. A solution of these equations is given in terms of the solution of a system of independent linear equations. Moreover, for zero external potential in the hard-rod system we specify various central regions between the confining walls, where the occupation probabilities are constant and the correlation functions are translationally invariant in the canonical ensemble. In the grand canonical ensemble such regions do not exist.

KEY WORDS: Density functional theory; nonuniform lattice gases; nonlinear difference equations; density correlations; confined systems; Takahashi interaction; hard rods.

1. INTRODUCTION

The understanding of the static and dynamic behavior of fluids in confined geometries is a problem of active current research.[1,2] This research is largely motivated by technological applications where one wants to create small surface structures with suitable physical and chemical properties.[3] The question, how the formation of such structures is influenced by confining walls, has raised the interest in many basic phenomena, such as the

[1] Fakultät für Physik, Universität Konstanz, D-78457 Konstanz, Germany.

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development of density profiles, pair correlations and ordering effects at surfaces,[4] wetting transitions,[5, 6] or a variety of surface induced kinetic processes.[7] In general, an exact analytical treatment of the various effects is not possible and one has to rely on approximation schemes. Well established techniques for this purpose are the density functional theory with its many variants (see ref. 8 and references therein), the cluster variation[9] and path probability method,[10] as well as the classical thermodynamic perturbation theories (see e.g., ref. 11). In one-dimensional fluid systems, however, exact results can be obtained for special models. Such results have their merits in establishing "boundary conditions" for the development of approximate theories in higher dimensions $d>1$ in the sense that these should become exact for $d=1$. Physically, this issue in particular pertains to theories for confined systems with tunable confinement, allowing a "dimensional crossover" from the case $d>1$ to $d=1$.[12] Exact findings also provide the possibility to systematically test the quality of approximations. Moreover, for many phenomena, such as e.g., the emergence of the well-known density oscillations of fluids near hard walls, the dimensionality does not seem to play a crucial role, and valuable insight into the origin of these phenomena may be gained by investigating appropriate one-dimensional reference systems.

The first exact density functional in $d=1$ was set up by Percus[13] for a fluid of hard rods. This functional yields an integral equation for the density profile in an arbitrary external potential. Later Percus showed that a further exact density functional can be written down for the special "sticky core" model[14] that, in addition to the hard-rod repulsion, includes a "zero-range" attractive force between nearest neighbor rods. This was subsequently generalized to finite-range forces between neighboring rods.[15] A generalized discrete version of the continuum hard-rod fluid on a linear chain was studied by Robledo and Varea.[16] They derived an exact functional for the mean occupation numbers of the rod centers on the chain, which, by taking the continuum limit, allowed them to recover the continuum density functional of Percus (for a review on classical density functionals, see ref. 17). Within this theory, the discrete hard-rod model leads to a rather complicated system of nonlinear finite difference equations for the mean occupation numbers in an arbitrary external potential, whose numerical solution requires a considerable computational effort.

In this article we will show that a more general discrete one-dimensional system can be considered, which allows one to calculate bulk and surface thermodynamical properties as well as equilibrium density profiles and density correlations in arbitrary external potentials. The system is an extension of the continuum Takahashi model[19] to a lattice gas model, in which only neighboring particles interact with each other. We first show that the canonical and grand canonical partition functions of this "Takahashi lattice gas" (TLG) obey simple recursion relations and that density profiles and density correlations can be conveniently calculated from the partition functions due to the one-dimensional nature of the model. Since the TLG contains as a special case the hard-rod model studied by Robledo and Varea[16] (for which the interaction potential would be infinite for interparticle distances smaller than the rod length and zero else), we can give a simple solution of the nonlinear difference equations derived in ref. 16. In this context we found it worthwhile to rederive the central formulae given in ref. 16. We will apply our formalism to a system of hard-rods confined both by hard and soft walls, and also to a system of particles, which in addition to the thermal hard-rod repulsion experience a finite interaction potential over a limited range. For these different cases density profiles and density correlations near the confining walls will be discussed in detail and compared with each other.

2. TAKAHASHI LATTICE GAS

In the TLG we consider N particles at positions i_k, $k=1,..., N$, on a linear chain with M sites $i=1,..., M$. No more than one particle is allowed to occupy a given lattice site. Two neighboring particles separated by $n-1$ vacant lattice sites interact via a potential $v(n)$. There is no interaction between particles that are not nearest neighbors, that means between particles that have at least one other particle in between them. In addition the particles experience an external potential $u(i)$ and it is assumed that two confining walls are present at the boundary sites $i=0$ and $i=M+1$. These are modeled by two additional particles that are held fixed at the boundary sites. The energy of a particle configuration $1 \leqslant i_1 < \cdots < i_N \leqslant M$ is then given by

$$\beta H = \sum_{k=1}^{N} u(i_k) + v(i_1) + \sum_{k=2}^{N} v(i_k - i_{k-1}) + v(M+1-i_N) \tag{2.1}$$

where $\beta = 1/k_B T$ and we have assumed for simplicity that the particles at the boundary sites are the same as those on the chain. It will become clear in the following that one could also consider a modified interaction with the walls.

2.1. General Case of Arbitrary External Potential

In the presence of a (non-constant) external potential $u(i)$, it is convenient to define a generalized canonical partition function by

$$Z(N, M', \alpha) = \sum_{1 \leqslant i_1 < \cdots i_N \leqslant M'} \exp -\left[\sum_{k=1}^{N} u(i_k + \alpha) + v(i_1) + \sum_{k=2}^{N} v(i_k - i_{k-1}) + v(M' + 1 - i_N) \right] \tag{2.2}$$

for integers $\alpha \geqslant 0$ and $M' + \alpha \leqslant M$. Equation (2.2) defines $Z(N, M', \alpha)$ if $N \leqslant M'$, while for $N > M'$ we set $Z(N, M', \alpha) \equiv 0$. Note that for $\alpha = 0$ and $M' = M$ we recover the ordinary partition function $Z(N, M) \equiv Z(N, M, 0)$. As far as only thermodynamic quantities shall be calculated, we could limit ourselves to the conventional form, but to evaluate density profiles and density correlations for the TLG, we need to consider the generalized functions (see below). Separating the summation over the positions $l = i_N$ of the rightmost particle, we can write

$$\begin{aligned} Z(N, M', \alpha) &= \sum_{l=N}^{M'} \exp[-v(M' + 1 - l) - u(l + \alpha)] \\ &\quad \times \sum_{1 \leqslant i_1 < \cdots < i_{N-1} \leqslant l-1} \exp -\left[\sum_{k=1}^{N-1} u(i_k + \alpha) + v(i_1) + \sum_{k=2}^{N-1} v(i_k - i_{k-1}) + v(l - i_{N-1}) \right] \\ &= \sum_{l=1}^{M'} \exp[-v(M' + 1 - l) - u(l + \alpha)]\, Z(N - 1, l - 1, \alpha) \end{aligned} \tag{2.3}$$

In the last line we could start the summation from $l = 1$ because of our setting $Z(N, M', \alpha) \equiv 0$ for $N > M'$. The recursion relation (2.3) is so far valid for $N > 1$. It becomes valid also for $N = 1$ if we set $Z(0, M', \alpha) \equiv \exp[-v(M' + 1)]$.

From Eq. (2.3) we readily derive a recursion relation for the analogous generalized grand partition function,

$$\begin{aligned} \Omega(\lambda, M', \alpha) &= \sum_{N=0}^{\infty} Z(N, M', \alpha)\, \lambda^N \\ &= \exp[-v(M' + 1)] \\ &\quad + \lambda \sum_{l=1}^{M'} \exp[-u(l + \alpha) - v(M' + 1 - l)]\, \Omega(\lambda, l - 1, \alpha) \end{aligned} \tag{2.4}$$

As before, we define $\Omega(\lambda, M) \equiv \Omega(\lambda, M, 0)$. This recursion relation (2.5) is valid for $M' > 1$, but can be made valid also for $M' = 1$ if we set $\Omega(\lambda, 0, \alpha) = \exp[-v(1)]$. The fugacity λ determines, for given M, the mean number $N(\lambda, M)$ of particles in the system.

Using the recursion relations (2.3, 2.4) one may calculate all thermodynamic properties for a given interaction $v(n)$ and external potential $u(i)$ by taking $\alpha = 0$ and $M' = M$. We now show how one can calculate also density profiles and correlations (of arbitrary order), once $Z(N, M', \alpha)$ or $\Omega(\lambda, M', \alpha)$ has been calculated from Eqs. (2.3, 2.4). To this end we first determine the probability $w(l, r)$ to find the rth particle at position $i_r = l$,

$$\begin{aligned}
w(l, r) = {} & Z^{-1}(N, M) \sum_{\cdots < i_{r-1} < l < i_{r+1} < \cdots} \exp -\Bigg[v(i_1) + \sum_{k=2}^{N} v(i_k - i_{k-1}) \\
& + v(M + 1 - i_N) + \sum_{k=1}^{N} u(i_k) \Bigg] \\
= {} & \exp[-u(l)]\, Z^{-1}(N, M) \\
& \times \sum_{1 \leqslant i_1 < \cdots < i_{r-1} \leqslant l-1} \exp -\Bigg[v(i_1) + \sum_{k=2}^{r-1} v(i_k - i_{k-1}) \\
& + v(l - 1 + 1 - i_{r-1}) + \sum_{k=1}^{r-1} u(i_k) \Bigg] \\
& \times \sum_{l+1 \leqslant i_{r+1} < \cdots < i_N \leqslant M} \exp -\Bigg[v(i_{r+1} - l) + \sum_{k=r+2}^{N} v(i_k - i_{k-1}) \\
& + v(M + 1 - i_N) + \sum_{k=r+1}^{N} u(i_k) \Bigg] \\
= {} & \exp[-u(l)]\, Z^{-1}(N, M)\, Z(r-1, l-1) \\
& \times \sum_{1 \leqslant j_1 < \cdots < j_{N-r} \leqslant M-l} \exp -\Bigg[v(j_1) + \sum_{k=2}^{N-r} v(j_k - j_{k-1}) \\
& + v(M - l + 1 - j_{N-r}) + \sum_{k=1}^{N-r} u(j_k + l) \Bigg] \\
= {} & \exp[-u(l)] \frac{Z(r-1, l-1)\, Z(N-r, M-l, l)}{Z(N, M)}
\end{aligned} \tag{2.5}$$

In the second step we have introduced the shifted particle positions $j_s = i_{r+s} - l$ for $s = 1,..., N - r$. By doing this, $u(i_k)$ transforms to $u(j_k + l)$ and it becomes clear now why we had to introduce the generalized partition function $Z(N, M', \alpha)$ with $\alpha \neq 0$. In the canonical ensemble the probability $p(l; N, M)$ for the site l to be occupied is then given by

$$p(l; N, M) = \sum_{r=1}^{N} w(l, r) = \frac{\exp[-u(l)]}{Z(N, M)} \sum_{r=1}^{N} Z(r-1, l-1)\, Z(N-r, M-l, l) \tag{2.6}$$

In the grand canonical ensemble the convolution in Eq. (2.6) factorizes and we obtain the corresponding occupation probability

$$\tilde{p}(l; \lambda, M) = \lambda \exp[-u(l)]\, \frac{\Omega(\lambda, l-1)\, \Omega(\lambda, M-l, l)}{\Omega(\lambda, M)} \tag{2.7}$$

We like to note that for a symmetric external potential, $u(i) = u(M+1-i)$, it follows that $\Omega(\lambda, M-l, l) = \Omega(\lambda, M-l)$. Hence it suffices to calculate $\Omega(\lambda, M', \alpha)$ from Eq. (2.4) for $\alpha = 0$ to obtain the density profile in this symmetric case.

By an analogous decomposition of the partition function into products of generalized partition functions (corresponding to various system sizes) one can derive the joint probabilities $p_s(l_1, ..., l_s; N, M)$ to find the sites $l_1 < \cdots < l_s$ being occupied in the canonical ensemble,

$$\begin{aligned} p_s(l_1, ..., l_s; N, M) = {} & \frac{\exp[-\sum_{k=1}^{s} u(l_k)]}{Z(N, M)} \\ & \times \sum_{1 \leqslant r_1 < \cdots < r_s \leqslant N} \Big\{ Z(r_1 - 1, l_1 - 1)\, Z(N - r_s, M - l_s, l_s) \\ & \times \prod_{k=1}^{s-1} Z(r_{k+1} - r_k - 1, l_{k+1} - l_k - 1, l_k) \Big\} \end{aligned} \tag{2.8}$$

From this we obtain the corresponding joint probabilities in the grand canonical ensemble,

$$\begin{aligned} \tilde{p}_s(l_1, ..., l_s; \lambda, M) = {} & \frac{\lambda^s \exp[-\sum_{k=1}^{s} u(l_k)]}{\Omega(\lambda, M)}\, \Omega(\lambda, l_1 - 1)\, \Omega(\lambda, M - l_s, l_s) \\ & \times \prod_{k=1}^{s-1} \Omega(\lambda, l_{k+1} - l_k - 1, l_k) \end{aligned} \tag{2.9}$$

Note that for $s = 1$ Eqs. (2.8), (2.9) reduce to Eqs. (2.6), (2.7). From Eqs. (2.6), (2.8) or Eqs. (2.7), (2.9) one can readily calculate density profiles and density correlations of arbitrary order in the canonical or grand canonical ensemble for arbitrary interaction $v(n)$ and external potential $u(i)$.

2.2. Special Case of Vanishing External Potential

In case of a vanishing (or constant) external potential it is not needed to introduce the generalized partition functions in Eqs. (2.2), (2.4) and accordingly one can set the third argument α in $\Omega(\lambda, M, \alpha)$ equal to zero in all formulae in Section 2.1. The occupation probabilities $p(l; N, M)$ and $\tilde{p}(l; \lambda, M)$ in Eqs. (2.6), (2.7) can be written as

$$\begin{aligned} p(l; N, M) &= \sum_{r=1}^{N} Z(r-1, l-1) \frac{Z(N-r, M-l)}{Z(N, M)} \\ \tilde{p}(l; \lambda, M) &= \lambda \frac{\Omega(\lambda, l-1)\, \Omega(\lambda, M-l)}{\Omega(\lambda, M)} \end{aligned} \tag{2.10}$$

and analogous simplifications are obtained for the joint probabilities of higher order in Eqs. (2.8) and (2.9).

Moreover, we can solve the recursion relations (2.3), (2.4) explicitly in terms of the generating functions $H(N, s) = \sum_{M=0}^{\infty} Z(N, M)\, s^M$ and $G(\lambda, s) = \sum_{M=0}^{\infty} \Omega(\lambda, M)\, s^M$, which are explicitly given by

$$H(N, s) = \frac{\varphi(s)^{N+1}}{s}, \qquad G(\lambda, s) = \frac{\varphi(s)}{s[1-\lambda\varphi(s)]} \tag{2.11}$$

with

$$\varphi(s) = \sum_{l=1}^{\infty} \exp[-v(l)]\, s^l \tag{2.12}$$

If $v(l)$ has a finite range, that means $v(l) = 0$ for $l \geqslant l_0$, we obtain from (2.11) $G(\lambda, s) = P(\lambda, s)/Q(\lambda, s)$, where $P(\lambda, s)$ and $Q(\lambda, s)$ are polynomials in s of degree to $l_0 - 1$ and l_0, respectively. According to a theorem for rational generating functions,[20] $\Omega(\lambda, M)$ then has the form $\Omega(\lambda, M) = \sum_{j=0}^{k} c_j(\lambda, M)\, s_j(\lambda)^{-M}$, where $s_j(\lambda)$, $j = 0,..., k$ are the distinct zeros of $Q(\lambda, s)$ with multiplicities d_j, and $c_j(\lambda, M)$ are polynomials in M of degree less than d_j. The moduli of the zeros s_j are considered to be ordered, $|s_0| \leqslant |s_1| \leqslant \cdots \leqslant |s_k|$.

As shown in Appendix A, s_0 is real with $0 < s_0 < 1$, $d_0 = 1$, and $|s_j| > s_0$ for $j = 1,..., k$. Hence we can write $\Omega(\lambda, M) = s_0^{-M}[c_0 + \sum_{j=1}^{k} c_j(M)(s_0/s_j)^M]$ and obtain

$$\Omega(\lambda, M) \sim c_0(\lambda)\, s_0(\lambda)^{-M} \tag{2.13}$$

in the thermodynamic limit $M \to \infty$. The one-to-one correspondence between the fugacity λ and the number density $\bar{p} = N(\lambda, M)/M$ in this limit follows from the relations (see Corollary A.1. in Appendix A)

$$\bar{p} = \varphi(s_0)/[s_0 \varphi'(s_0)], \qquad \lambda = 1/\varphi(s_0) \tag{2.14}$$

Using the asymptotic limit for $\Omega(\lambda, M)$ we obtain from Eq. (2.10)

$$p_\infty(l; \lambda) \equiv \lim_{M \to \infty} \tilde{p}(l; \lambda, M) = \lambda \Omega(\lambda, l-1)\, s_0^l \tag{2.15}$$

In fact, as shown in Appendix A, Eqs. (2.14), (2.15) hold true even for a more general interaction potential $v(l)$, which for l larger than some l_* is bounded and for $l \to \infty$ approaches zero. The analogous occupation probability $p_\infty(l)$ in the canonical ensemble is the same as $p_\infty(l; \lambda)$, if for given $\bar{p}$ the corresponding unique fugacity λ is used (see Eq. (2.14) and Appendix A). Moreover, the joint probabilities $\tilde{p}_s(l_1,..., l_s; \lambda, M)$ in the grand-canonical ensemble (and the corresponding $p_s(l_1,..., l_s; N, M)$ in the canonical ensemble) factorize in terms of $p_\infty(l; \lambda)$ in the thermodynamic limit, that means

$$p_{s,\infty}(l_1,..., l_s; \lambda) \equiv \lim_{M \to \infty} \tilde{p}_s(l_1,..., l_s; \lambda, M) = p_\infty(l_1; \lambda) \prod_{k=2}^{s} p_\infty(l_k - l_{k-1}; \lambda) \tag{2.16}$$

For the special case of a finite range interaction potential considered above (i.e., $v(l) = 0$ for $l \geqslant l_0$) there exists a constant $C > 0$ such that $|p_\infty(l; \lambda) - \bar{p}| < Cl^\nu e^{-l/\xi}$, where $\nu \leqslant l_0 - 2$ is an integer, and $\xi = -1/\ln(r)$ with $r = \max_{1 \leqslant j \leqslant k} \{s_0/|s_j|\} < 1$.

3. HARD-ROD LATTICE GAS REVISITED

A particularly simple situation occurs, when the interaction potential in Eq. (2.1) is given by

$$v(n) = v_{\mathrm{HR}}(n) \equiv \begin{cases} \infty, & 0 \leqslant n < 2m \\ 0, & n \geqslant 2m \end{cases} \tag{3.1}$$

This potential can be viewed as describing a system composed of hard-rods with lengths $2m$ (with hard walls at positions m and $M+1-m$ due to the fixed hard-rods at positions 0 and $M+1$).

Setting the mass density of the rods equal to unity, we can express the local mass density $p_{\mathrm{mass}}(l; N, M)$ along the one-dimensional chain by the occupation probabilities $p(l; N, M)$ (that refer to the rod centers) according to

$$p_{\mathrm{mass}}(l; N, M) = \tfrac{1}{2}[p(l-m; N, M) + p(l+m; N, M)] + \sum_{j=-(m-1)}^{m-1} p(l-j; N, M) \tag{3.2}$$

This formula holds true in the canonical as well as in the grand canonical ensemble (if $p_{\mathrm{mass}}(l; N, M)$ is replaced by $\tilde{p}_{\mathrm{mass}}(l; \lambda, M)$ and $p(l; N, M)$ by $\tilde{p}(l; \lambda, M)$). Note that the total number N of rods must be smaller than $M/2m$.

3.1. Explicit Results for Homogeneous Systems

Density profiles and density correlations can be calculated explicitly in the absence of an external potential by using the general method developed in Section 2.2. From Eqs. (2.11) and (3.1) we find $\varphi(s) = s^{2m}/(1-s)$ and $G(\lambda, s) = s^{2m-1}/(1-s-\lambda s^{2m})$, and therefore

$$\begin{aligned} \Omega(\lambda, l) &= \sum_{n=0}^{\infty} \binom{l-(2m-1)(n+1)}{n} \lambda^n \\ Z(N, l) &= \binom{l-(2m-1)(N+1)}{N} \end{aligned} \tag{3.3}$$

The occupation probabilities $p(l; N, M)$ and $\tilde{p}(l; \lambda, M)$ in the canonical and grand-canonical ensemble then follow by inserting these expressions into Eq. (2.10), and the correlations analogously. One can show[18] that $p(l; N, M)$ and $\tilde{p}(l; \lambda, M)$ become maximal at the points $l = 2m$ and $l = M+1-2m$ closest to the walls. The reason for this is that by fixing the position of a rod next to a wall the number of possible configurations (and hence the entropy) for the remaining $(N-1)$ rods will be largest.

Extending this line of thinking one would guess that the most likely configuration near a wall is that where the rods are at positions $l = 2m$, $4m$, $6m$,.... One then should expect oscillations in the occupation probabilities to emerge with a period of typical size $2m$. In fact, in the thermodynamic limit $M \to \infty$ one finds $\lambda = 1/\varphi(s_0) = (1 - s_0)\, s_0^{-2m}$ with $s_0 = (1 - 2m\bar{p})/[1 - (2m-1)\,\bar{p}]$ (see Eq. (2.14)). Moreover, as shown in Appendix B, the zeros $s_j = |s_j| \exp(i\theta_j)$ (see Section 2.2) are all different, and Eq. (2.15) becomes

$$p_\infty(l, \lambda) = \bar{p} + \sum_{j=1}^{2m-1} c_j(\lambda) \left(\frac{s_0}{|s_j|}\right)^l e^{-i\theta_j l} \tag{3.4}$$

The θ_j are in the open interval $0 < \theta_j < 2\pi$, that means the profile $p_\infty(l, \lambda)$ is a superposition of simple oscillating and exponentially decaying functions. When considering a system of finite length, the effects induced by the second wall at position $M + 1 - m$ on the profile near the first wall at position m are of order l/M in the grand-canonical ensemble and of order l^2/M in the canonical ensemble. This is proven in Appendix B (more precisely, l must be of order $o(M^{1/2})$ in the canonical and of order $o(M)$ in the grand-canonical ensemble to obtain vanishing contributions in the thermodynamic limit.) Hence, the finite size corrections to Eq. (3.4) become small for large M. More surprising, if the number density is smaller than half of that for the closed packed configuration, i.e., $\bar{p} < 1/4m$, one can show (see Appendix B) that in the canonical ensemble the $p(l; N, M)$ are constant (l-independent) inside the central region $\mathscr{R}_1 \equiv \{l_1 \in \mathbb{N} \mid l^{(1)} \leqslant l_1 \leqslant M + 1 - l^{(1)}\}$ with $l^{(1)} \equiv (2m-1)\, N + 1$. At the outer boundary points $l^{(-)} \equiv l^{(1)} - 1$ and $l^{(+)} \equiv M + 2 - l^{(1)}$, $p(l^{\mp}; N, M)$ is different from the constant value inside $\mathscr{R}_1$, that means $\mathscr{R}_1$ is "maximal" in the sense that there exits no other region of constant occupation probability enclosing parts of $\mathscr{R}_1$. It is interesting to note that $|p(l^{(\mp)} \pm 1; N, M) - p(l^{(\mp)}; N, M)| = 1/Z(N, M)$, that means the logarithm of the jump in the occupation probability at the boundaries of $\mathscr{R}_1$ provides the free energy $\propto \log Z(N, M)$. Furthermore, the joint probabilities $p_s(l_1,..., l_s; N, M)$ are translationally invariant inside ("maximal") regions $\mathscr{R}_s \equiv \{(l_1,..., l_s) \in \mathbb{N}^s) \mid l^{(s)} < l_1;\ 2m \leqslant l_k - l_{k-1}$ for $k = 2,..., s;\ l_s \leqslant M + 1 - l^{(s)}\}$ with $l^{(s)} = (2m-1)(N + 1 - s) + 1$,[2] that means there exists a function $f(x_1,..., x_{s-1}; N, M)$ such that for all $(l_1,..., l_s) \in \mathscr{R}_s$, $p_s(l_1,..., l_s; N, M) = f(l_2 - l_1,..., l_s - l_{s-1}; N, M)$. Corresponding regions have been found in the continuum version of the hard-rod lattice gas, the so-called hard-core fluid model.[21] Moreover, if $(l_{j+1} - l_j) \geqslant [(2m-1)(N + 1 - s) + 1]$ for all $j = 1,..., s-1$, then $p_s(l_1,..., l_s; N, M)$ is constant for $(l_1,..., l_s) \in \mathscr{R}_s$ (this was shown to hold true in the continuum model for the pair distribution functions only[22]). As is shown in Appendix B also, the situation is quite different in the grand-canonical ensemble. Here, there exist no regions of constant occupation probabilities and translational invariance of the joint probabilities (except for trivial cases[2]).

3.2. Free Energy Functional

An alternative way to treat the hard-rod lattice gas has been followed in ref. 16. In this approach, which relates to density functional theory of classical fluids, one considers the grand-canonical ensemble and defines the occupation numbers x_i, where $x_i = 1$ if site i is occupied by a rod center, and $x_i = 0$ else.[3] Note that these random variables are not independent: Since the rods have size $2m$ we have to require $x_j = 0$ for $|j-i| < 2m$ if $x_i = 1$. We define $\mathscr{C}_M$ as the set of all allowed configurations $\{x_i\}$. The idea then is to calculate explicitly the probability $\chi(x_1,..., x_M)$ of an allowed configuration $(x_1,..., x_M) \in \mathscr{C}_M$ by regarding the occupation probabilities $\tilde{p}_i = \langle x_i \rangle$ as fixed ($\langle [\cdots] \rangle \equiv \sum_{(x_1,..., x_M) \in \mathscr{C}_M} [\cdots] \, \chi(x_1,..., x_M)$). For given $\tilde{p}_i$ it turns out that $\log \chi(x_1,..., x_M)$ depends linearly on the occupation numbers (which is a fortunate feature of the hard rod system, see below). By equating $\chi(x_1,..., x_M)$ with the Boltzmann formula for all $(x_1,..., x_M) \in \mathscr{C}_M$ we have

$$-\log \Omega(\lambda, M) = \log \chi(x_1,..., x_M) + \sum_{s=1}^{M} x_s[u(s) - \mu] \qquad (3.5)$$

where $\mu = \log \lambda$ is the chemical potential. Taking now the expectation value of (3.5) with respect to the x_i, an exact density functional $\beta\mathscr{F}(\tilde{p}_1,..., \tilde{p}_M) = -\log \Omega(\lambda, M)$ of the $\tilde{p}_i$ is obtained.

In order to determine $\chi(x_1,..., x_M)$ for $(x_1,..., x_M) \in \mathscr{C}_M$ we will make use of a Markov property (that is valid only in the grand-canonical ensemble). The constraint given by the finite rod lengths implies that the conditional probabilities $w_s(x_s \mid x_{s-1},..., x_1)$ for the occupation number at site s to be x_s, given $x_{s-1},..., x_1$, are independent of $x_1,..., x_{s-2m}$. In other words

[2] By saying that the $p_s(l_1,..., l_s; N, M)$ are not translationally invariant if $l_1 < \cdots < l_s \notin \mathscr{R}_s$ we exclude the trivial case, where l_1 and l_s *must* be occupied by the first and last rod center, respectively (i.e. for $l_1 < 4m$ and $l_s > M + 1 - 4m$). In this case, our system can be considered as being composed of $N-2$ rods on a chain of length $(l_s - l_1)$ and the $p_s(l_1,..., l_s; N, M)$ are translationally invariant then on trivial reasons.

[3] For the following it is convenient to make the transformation $l \to l - (2m-1)$ of the site positions and to change the system size according to $M \to M + 4m - 2$. After these replacements the rods at the boundaries are at positions $-2m+1$ and $M + 2m$ corresponding to hard walls at positions -$m+1$ and $M + m$. Accordingly, the possible positions of the rod centers are 1,..., M.

$w_s(x_s \mid x_{s-1},..., x_1)$ fulfills the generalized Markov condition (which is rather obvious here but can be proven rigorously too[18])

$$w_s(x_s \mid x_{s-1},..., x_1) = w_s(x_s \mid x_{s-1},..., x_{s-2m+1}) \tag{3.6}$$

Due to this property we can express the joint probabilities $\chi(x_1,..., x_M)$ as

$$\chi(x_1,..., x_M) = w_1(x_1)\, w_2(x_2 \mid x_1) \cdots w_{2m}(x_{2m} \mid x_{2m-1},..., x_1) \cdots \\ \times w_s(x_s \mid x_{s-1},..., x_{s-2m+1}) \cdots w_M(x_M \mid x_{M-1},..., x_{M-2m+1}) \tag{3.7}$$

It is convenient to formally extend the system to integers $i \leqslant 0$ and to set $x_i = 0$ for all $-2m+2 \leqslant i \leqslant 0$, such that we can write Eq. (3.7) in the compact form

$$\chi(x_1,..., x_M) = \prod_{s=1}^{M} w_s(x_s \mid x_{s-1},..., x_{s-2m+1}) \tag{3.8}$$

For calculating $w_s(x_s \mid x_{s-1},..., x_{s-2m+1})$ we have to deal with two cases only: (i) One of the given random variables $x_{s-2m+1},..., x_{s-1}$ is equal to one and the rest of them equal to zero, and (ii) all $x_{s-2m+1},..., x_{s-1}$ are zero. In all other cases there would be at least two of the $x_{s-2m+1},..., x_{s-1}$ equal to one, but this is not allowed, because it would imply that rods overlap. For the same reason we must have $x_s = 0$ in situation (i), that means we obtain

$$w_s(x_s = 0 \mid x_{s-1} = 0,..., x_i = 1,..., x_{s-2m+1} = 0) = 1 \tag{3.9}$$

The situation (ii) is more complicated. By definition we can write

$$w_s(x_s \mid 0,..., 0) = \frac{\kappa_{s,\, s-2m+1}(x_s,\, x_{s-1} = 0,..., x_{s-2m+1} = 0)}{\kappa_{s-1,\, s-2m+1}(x_{s-1} = 0,..., x_{s-2m+1} = 0)} \tag{3.10}$$

where $\kappa_{l,\,k}(x_l,..., x_k)$ is the joint probability for the configuration $\{x_l,..., x_k\}$ to occur. For $k - l < 2m$ the normalization condition yields (again because of the non-overlapping condition)

$$1 = \sum_{\{x_j\}} \kappa_{l,\,k}(x_l,..., x_k) = \kappa_{l,\,k}(0,..., 0) + \sum_{j=k}^{l} \kappa_{l,\,k}(0,..., x_j = 1,..., 0) \tag{3.11}$$

By definition we further have (for $k - l < 2m$)

$$\tilde{p}_i = \sum_{\{x_j\}} x_i \kappa_{l,\,k}(x_l,..., x_k) = \kappa_{l,\,k}(0,..., x_i = 1,..., 0) \tag{3.12}$$

and hence it follows form Eqs. (3.11), (3.12),

$$\kappa_{l,k}(0,..., 0) = 1 - \sum_{j=k}^{l} \tilde{p}_j \tag{3.13}$$

Inserting the $\kappa_{l,k}(x_l,..., x_k)$ from Eqs. (3.12), (3.13) into Eq. (3.10), we obtain

$$w_s(x_s \mid 0,..., 0) = \begin{cases} \dfrac{1 - t_m(s)}{1 - t'_m(s)}, & x_s = 0 \\ \dfrac{\tilde{p}_s}{1 - t'_m(s)}, & x_s = 1 \end{cases} \tag{3.14}$$

where we have defined $t_m(s) = \sum_{j=0}^{2m-1} \tilde{p}_{s-j}$ and $t'_m(s) = \sum_{j=1}^{2m-1} \tilde{p}_{s-j} = t_m(s) - \tilde{p}_s$. The results (3.9), (3.14) can be combined to express $w(x_s \mid x_{s-1},..., x_{s-2m+1})$ in the general form

$$w(x_s \mid x_{s-1},..., x_{s-2m+1}) = \tilde{p}_s^{x_s} \frac{[1 - t_m(s)]^{(1 - \Sigma_{j=0}^{2m-1} x_{s-j})}}{[1 - t'_m(s)]^{(1 - \Sigma_{j=1}^{2m-1} x_{s-j})}} \tag{3.15}$$

Note that the x_i appear linearly in the exponents of the transition matrix (3.15), such that by inserting (3.15) into Eq. (3.8), and taking the logarithm, we find that $\log \chi$ is *linear* in the x_i. Using Eq. (3.5) and averaging over x_i we finally obtain[16]

$$\begin{aligned} \beta\mathscr{F}(\tilde{p}_1,..., \tilde{p}_M) = {} & \sum_{s=1}^{M} \tilde{p}_s[u(s) - \mu] + \sum_{s=1}^{M} \tilde{p}_s \log \tilde{p}_s \\ & + \sum_{s=1}^{M} (1 - t_m(s)) \log(1 - t_m(s)) \\ & - \sum_{s=1}^{M} (1 - t'_m(s)) \log(1 - t'_m(s)) \end{aligned} \tag{3.16}$$

The functional (3.16) becomes minimal for the equilibrium density profile $\tilde{p}_l \equiv \tilde{p}(l; \lambda, M)$. The corresponding system of equations reads $(l = 1,..., M)$

$$\begin{aligned} \frac{\partial(\beta\mathscr{F})}{\partial\tilde{p}_l}(\tilde{p}_1,..., \tilde{p}_M) = {} & -\mu + u(l) + \log \tilde{p}_l + \sum_{s=l+1}^{l+2m-1} \log(1 - t'_m(s)) \\ & - \sum_{s=l}^{l+2m-1} \log(1 - t_m(s)) = 0 \end{aligned} \tag{3.17}$$

It is clear that $\tilde{p}(l; \lambda, M)$ from Eq. (2.7) (after making the transformations $l \to l-(2m-1)$ and $M \to M+2-4m$) must solve (3.17). From a mathematical point of view this is an interesting example, where a system of coupled nonlinear difference equations (Eq. (3.17)) can be mapped by a nonlinear transformation (Eq. (2.7)) onto a simple system of independent linear difference equations (Eq. (2.4)). For the special case of a vanishing external potential even an explicit solution exists (see Eqs. (2.10), (3.3)). A direct proof that $\tilde{p}(l; \lambda, M)$ from (2.7) indeed solves (3.17) is given in Appendix C.

Next we rederive the exact free energy functional of Percus[13] by taking the proper continuum limit of Eq. (3.16). To do this we first have to note that Eq. (3.16) gets slightly modified, when it is viewed as resulting from a discretized form of an originally continuous system. This continuous system is defined by hard rods of length σ with positions $0 < y_i < L$, $y_{i+1} - y_i \geqslant \sigma$. In a discretization, we may subdivide the continuous system into M intervals $\mathscr{I}_s$ $(s = 1,..., M)$ of equal size $\Delta y = L/M$, and may set the rod length $2m$ in the new discrete variables s equal to the integer part of $\sigma L/M$. The occupation number x_s of the interval $\mathscr{I}_s$ is defined to be zero, if none of the $y_i \in \mathscr{I}_s$ and one else. Then the joint probability $q(i_1,..., i_N)$ to find N rods at positions $y_1,..., y_N$ in the intervals $\mathscr{I}_{i_1},..., \mathscr{I}_{i_N}$ is,

$$\begin{aligned} q(i_1,..., i_N) &= \Omega(\lambda, L)^{-1} \prod_{k=1}^{N} \int_{\mathscr{I}_{i_k}} dy_k \exp(-[u(y_k) - \mu]) \\ &= \Omega(\lambda, L)^{-1} (\Delta y)^N \exp\left(-\sum_{k=1}^{N} [u(i_k) - \mu]\right) \left[1 + \frac{o(\Delta y)}{\Delta y}\right] \end{aligned} \tag{3.18}$$

Since there is a one-to-one correspondence between the sets $\{i_1,..., i_N\}$ and $\{x_1,..., x_M\}$ we immediately obtain

$$\chi(x_1,..., x_M) = \Omega(\lambda, L)^{-1} (\Delta y)^{\sum_{s=1}^{M} x_s} \exp\left(-\sum_{s=1}^{M} [u(s) - \mu] x_s\right) \left[1 + \frac{o(\Delta y)}{\Delta y}\right] \tag{3.19}$$

Repeating the steps leading to Eq. (3.16) we get a modified functional $\mathscr{F}(\tilde{p}_1,..., \tilde{p}_M)$, which is the same as given in (3.16) plus the term $[-(\sum_s \tilde{p}_s) \log \Delta y + o(\Delta y)/\Delta y]$. The $\tilde{p}_s$ are related to the occupation number density $\rho(y)$ in the continuous system by $\tilde{p}_s = \int_{\mathscr{I}_s} dy\, \rho(y) = [\rho(sL/M)\, \Delta y + o(\Delta y)]$ and by inserting this in the modified form of Eq. (3.16) we obtain in the limit $M \to \infty$ $(\Delta y \to 0)$ the Percus functional

$$\beta \mathscr{F}[\rho] = \int_0^L dy\, \rho(y)\{u(y) - \mu + \log \rho(y) - [1 + \log(1 - t(y))]\} \tag{3.20}$$

where $t(y) = \int_{y-\sigma}^{y} dz\, \rho(z)$. To consider Eq. (3.20) as a mass density functional one should remember the relation $\rho_{\text{mass}}(y) = t(y+\sigma/2) = \int_{y-\sigma/2}^{y+\sigma/2} dz\, \rho(z)$ between the mass and the number density (that might be easily inverted by Laplace transformation).

4. DENSITY PROFILES AND PAIR CORRELATIONS NEAR WALLS

In this section we calculate density profiles and correlations for some cases to exemplify the formalism developed in the previous Sections 2 and 3.

Figure 1 shows the occupation probability $p_\infty(l)$ for a system of hard rods as a function of the distance l from a hard wall for (a) $\bar{p} = 0.1$ and various (half) rod lengths $m = 2, 3, 4$, and (b) $\bar{p} = 0.02$ and $m = 14, 18$, and 22 ($p_\infty(l)$ was calculated from Eqs. (2.4, 2.15)). As can be seen from the figure, $p_\infty(l)$ exhibits oscillations with a period of order $2m$, which become more pronounced with increasing m. For large l, $p_\infty(l)$ approaches $\bar{p}$. Note that for $\bar{p} = 0.1$ the closed packed situation occurs already at $m = 5$ and the discreteness of the system is important (see Fig. 1a), while $\bar{p} = 0.02$ (Fig. 1b) corresponds to a continuum situation. The data in Fig. 1b indicate that $p_\infty(l)$ in the continuum limit (see Sect. 3.2) might have a discontinuity in the first derivative at the first minimum. Indeed this discontinuity occurs and its origin can be understood from the solution of the discrete system: From Eq. (2.15) and the recursion relation (2.4) one derives

$$p_\infty(l) = s_0 p_\infty(l-1) + (1-s_0)\, p_\infty(l-2m) \tag{4.1}$$

Accordingly, when $l < 4m$, the second term in (4.1) is zero up to the first minimum in $p_\infty(l)$ at $l = 4m-1$, and it first contributes when $l = 4m$. The additional contribution from the second term yields the discontinuity in the first derivative.

The correlation function

$$C(l) \equiv p_{2,\infty}(2m, l) - p_\infty(2m)\, p_\infty(l) \tag{4.2}$$

between the first possible position $2m$ of a rod center and another rod center that is at distance l from the wall is shown in Fig. 2 for the same parameters as in Fig. 1. Similar as $p_\infty(l)$, $C(l)$ oscillates as a function of l with a period of order $2m$; the strength of the oscillations increases with increasing m. For large l, the absolute values of $C(l)$ at its local maxima and minima decrease exponentially with l.

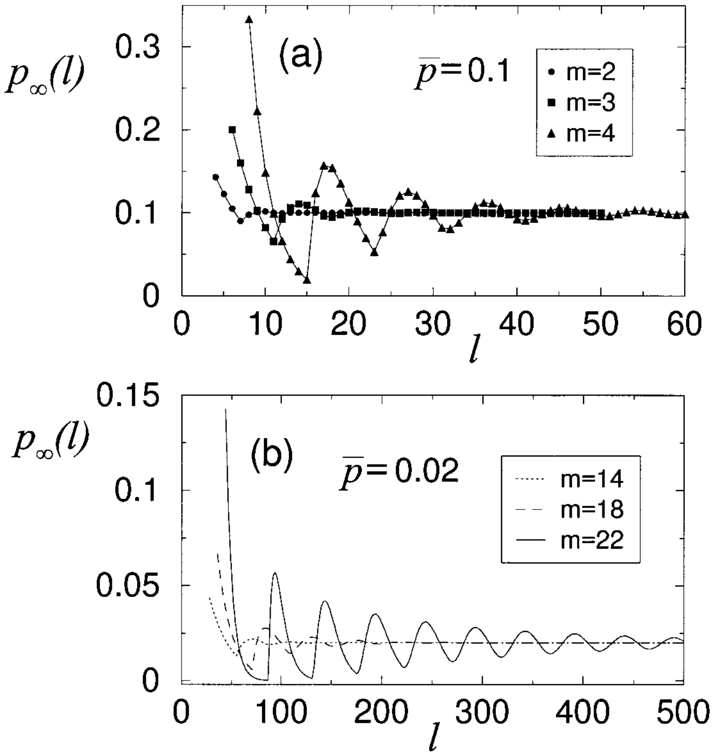

Fig. 1. Occupation probability $p_\infty(l)$ of hard rod centers as a function of the distance l from a hard wall for (a) three small rod lengths and a large number density $\bar{p} = 0.1$, and (b) three large rod lengths and a small mean occupation number $\bar{p} = 0.02$ corresponding to a continuum-like situation. The solid lines in (a) were drawn as a guide for the eye.

Next we calculate density profiles and correlations for more general cases. To this end we consider (i) hard rods ($v(l) = v_{\mathrm{HR}}(l)$) in the presence of a "soft wall" with an attractive potential

$$\beta u_0(l) \equiv -5 \exp(-l/20) \tag{4.3}$$

and (ii) particles with a Lennard–Jones type Takahashi interaction of the form

$$\beta v_{\mathrm{LJ}}(l) \equiv \begin{cases} \infty & l < 2m \\ -4 & 2m \leqslant l \leqslant 3m \\ 0 & \text{else} \end{cases} \tag{4.4}$$

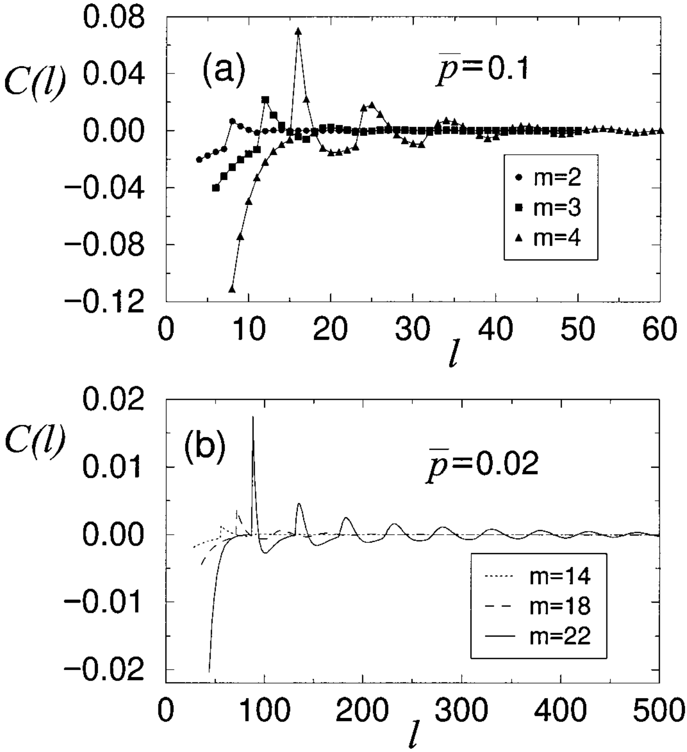

Fig. 2. Correlation function $C(l)$ between the first possible position $2m$ of a rod center and another rod center that is at distance l from the wall (see Eq. 4.2)) for the same parameters as in Figs. 1a, b. The solid lines in (a) were drawn as a guide for the eye.

in the presence of a hard wall ($u(l)=0$). Figure 3 shows $p_\infty(l)$ for these two cases in comparison with the hard rod system for (a) $m=4$ and (b) $m=18$ (to calculate $p_\infty(l)$ for $u(l)=u_0(l)$ we have chosen a large system size $M=10^4$ and used Eqs. (2.4), (2.7)). For both cases oscillations occur similar as in the hard rod system. In Fig. 3a the attractive wall potential causes the maxima and minima to become more pronounced than in the other cases, while in Fig. 3b only the occupation probability for the first rod next to the wall is strongly enhanced. Because the first rod center is strongly attracted by the wall, the position of the following minima and maxima of p_∞ are shifted toward the wall. The weaker effects of the external potential in the continuum-like situation (Fig. 3b) are due to the fact that the first minimum of $p_\infty(l)$ occurs at a position, where $u_0(l)$ is already very small. For the Lennard–Jones type interaction we find the oscillations in Fig. 3a to be stronger than in the hard rod system, but the probability

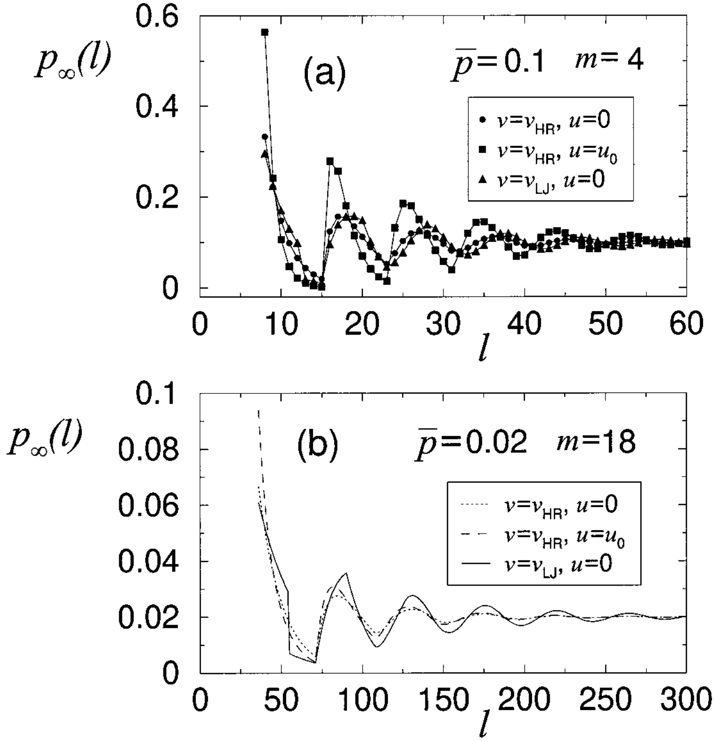

Fig. 3. Occupation probability $p_\infty(l)$ of rod centers as a function of the distance l from a wall for (i) hard rods in the presence of a hard wall ($v = v_{\mathrm{HR}}$, $u = 0$), (ii) hard rods in the presence of a soft wall ($v = v_{\mathrm{HR}}$, $u = u_0$), and (iii) rods with a Lennard–Jones type Takahashi interaction in the presence of a hard wall ($v = v_{\mathrm{LJ}}$, $u = 0$). In (a) the discrete nature of the lattice is important ($m = 4$, $\bar{p} = 0.1$), while in (b) the data correspond to a continuum-like situation ($m = 18$, $\bar{p} = 0.02$). The solid lines in (a) were drawn as a guide for the eye.

of the first rod to be right at the wall is reduced (for smaller m, however, $p_\infty(2m)$ can be larger than in the hard rod system). As can be seen from Figs. 4a, b, the changes of the correlation functions caused by the external potential $u_0(l)$ and by the interaction potential $v_{\mathrm{LJ}}(l)$ are fully analogous to the changes found for $p_\infty(l)$ in Figs. 3a, b.

5. SUMMARY

As demonstrated in Section 4, the recursion relations derived in Section 2 provide an efficient method to determine density distributions and correlations in the Takahashi lattice gas for arbitrary interactions and external potentials. We have proven in Appendix A that the wall-induced

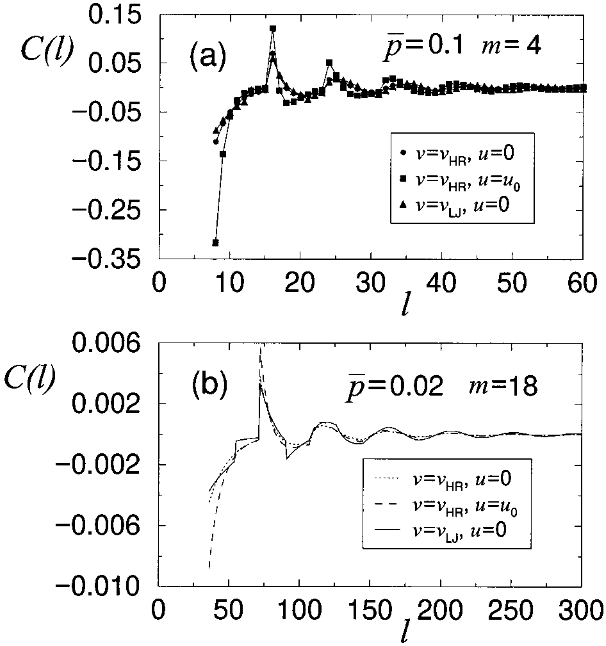

Fig. 4. Correlation function $C(l)$ between the first possible position $2m$ of a rod center and another rod centered that is at distance l from the wall (see Eq. (4.2)) for the same parameters as in Figs. 3a, b. The solid lines in (a) were drawn as a guide for the eye.

density oscillations decay exponentially into the bulk, if the interaction potential has a finite range. If the potential has no finite range but still decays to zero when the inter-particle distance increases toward infinity, one can show only that the density for large distances from the wall converges to a constant bulk value.

In the special case of the hard rod lattice gas, we have rederived the exact free energy functional of the occupation probabilities and the associated nonlinear system of coupled nonlinear difference equations. The general formalism derived in Section 2 allowed us to give a solution of these nonlinear difference equations in terms of the solution of a system of independent linear equations. Furthermore, various central regions between the confining walls have been specified in the canonical ensemble, where the occupation probabilities are constant, and where the correlations functions are translationally invariant or even constant too. In the grand canonical ensemble it was shown that such regions do not exist (except for trivial cases, see above).

It is possible to extend the calculations for the hard rod system to more general situations, as, for example, to systems where certain groups of particles have differing rod lengths, or even to systems with randomly distributed rod lengths.

APPENDIX A

For $|s|<1$ and $\lambda\in(0,\infty)$ the generating functions of the canonical and grandcanonical partition functions are (compare with Eq. (2.11))

$$\begin{aligned} H(N,s) &= \sum_{M=0}^{\infty} Z(N,M)\, s^M = \frac{\varphi(s)^{N+1}}{s} \\ G(\lambda,s) &= \sum_{M=0}^{\infty} \Omega(\lambda,M)\, s^M = \frac{\varphi(s)}{s[1-\lambda\varphi(s)]} \end{aligned} \tag{A.1}$$

with

$$\varphi(s) = \sum_{l=1}^{\infty} \exp[-v(l)]\, s^l \tag{A.2}$$

where $v(l)$ has the following properties

$$\begin{aligned} &\text{(i)} \quad \max_{l_*\leqslant l<\infty} |v(l)|<\infty \qquad \text{for some} \quad l_*<\infty \\ &\text{(ii)} \quad \lim_{l\to\infty} v(l)=0 \end{aligned} \tag{A.3}$$

Lemma A.1 (See also ref. 24). For given $\lambda\in(0,\infty)$, there exists exactly one real positive solution $s_0(\lambda)\in(0,1)$ of $1-\lambda\varphi(s)=0$ and this root is simple. If $s_j\in\mathbb{C}$ is another root of $1-\lambda\varphi(s)=0$, then $|s_j|>s_0$.

Proof. The series $\sum_{l=1}^{\infty}|\exp[-v(l)]\, s^l|$ converges for $|s|<1$, and accordingly $\varphi'(s)=\sum_{l=1}^{\infty} l\exp[-v(l)]\, s^{l-1}>0$ for positive real s. Since $\varphi(0)=0$ and $\varphi(1)=\infty$, there exists exactly one $s_0\in(0,1)$, for which $\varphi(s_0)=1/\lambda$ (with multiplicity one). If s_j were another root of $1-\lambda\varphi(s)=0$ with $|s_j|<s_0$, then $|\varphi(s_j)|\leqslant\varphi(|s_j|)<\varphi(s_0)=1/\lambda=\varphi(s_j)$, which is impossible. If $s_j=s_0\exp(i\theta)$ with $\theta\in(0,2\pi)$ we have to require $\sum_{l=1}^{\infty}\exp[-v(l)]\, s_0^l\,[1-\cos(l\theta)]=0$ and hence $\theta=2\pi k$, $k\in\mathbb{Z}$, in contradiction to the assumption $\theta\in(0,2\pi)$.

Theorem A.1. Let $s_0(\lambda)\in(0,1)$ be the unique real positive solution of $1-\lambda\varphi(s)=0$. Then

$$\Omega(\lambda,M)\sim c_0(\lambda)\, s_0(\lambda)^{-M}, \qquad \text{for} \quad M\to\infty \tag{A.4}$$

where $c_0(\lambda)=\varphi(s_0)^2/s_0^2\varphi'(s_0)$.

Proof. Let $a_k \equiv \Omega(\lambda, k-1)\, s_0^k$ and $f_k \equiv \exp[-v(k)]\, s_0^k / \sum_{l=1}^{\infty} \exp[-v(l)]\, s_0^l$, for $k = 1, 2,...$, and set $\lambda = 1/\varphi(s_0)$. Then, according to Eq. (2.4),

$$a_M = \varphi(s_0)\, f_M + \sum_{l=1}^{M-1} f_{M-l} a_l = \sum_{l=1}^{M} a_{M-l} f_l \tag{A.5}$$

where $a_0 \equiv \varphi(s_0)$. Obviously, $f_l \geqslant 0$ and $\sum_{l=1}^{\infty} f_l = 1$. By employing the renewal theorem[25] it follows

$$a_M \sim \frac{a_0}{\sum_{l=1}^{\infty} l f_l} \qquad \text{for} \quad M \to \infty \tag{A.6}$$

Since $\sum_{l=1}^{\infty} l f_l = s_0 \varphi'(s_0)/\varphi(s_0)$, we obtain $\Omega(\lambda, M) = a_{M+1} s_0^{-(M+1)} \sim \varphi(s_0)^2\, s_0^{-M} / s_0^2 \varphi'(s_0) = c_0(\lambda)\, s_0^{-M}$ for $M \to \infty$.

Corollary A.1.

(i) $p_\infty(l; \lambda) \equiv \lim_{M \to \infty} \tilde{p}(l; \lambda, M) = \lambda \Omega(\lambda, l-1)\, s_0^l$

(ii) $p_{s,\infty}(l_1,..., l_s; \lambda) \equiv \lim_{M \to \infty} \tilde{p}_s(l_1,..., l_s; \lambda, M) = p_\infty(l_1; \lambda) \prod_{k=2}^{s} p_\infty (l_k - l_{k-1}; \lambda)$

(iii) $\bar{p} = \varphi(s_0)/s_0 \varphi'(s_0)$, where $\bar{p} = \lim_{M \to \infty} N(\lambda, M)/M$. ($N(\lambda, M)$ is the mean number of particles for given fugacity λ and M.)

Proof. According to Eq. (2.10), $\tilde{p}(l; \lambda, M) = \lambda \Omega(\lambda, l-1)\, \Omega(\lambda, M-l)/\Omega(\lambda, M)$ such that $\tilde{p}(l; \lambda, M) \sim \lambda \Omega(\lambda, l-1)\, c_0(\lambda)\, s_0^{-(M-l)}/c_0(\lambda)\, s_0^{-M} = \lambda \Omega(\lambda, l-1)\, s_0^l$ by Theorem A.1. In particular, $p_\infty(l; \lambda) = \lambda \Omega(\lambda, l-1)\, s_0^l$. Analogously, using Eq. (2.9), $p_{s,\infty}(l_1,..., l_s; \lambda) = \lambda^s \Omega(\lambda, l_1 - 1) \prod_{k=2}^{s} \Omega(\lambda, l_k - l_{k-1} - 1)\, s_0^{l_s}$. Since $l_s = l_1 + \sum_{k=2}^{s} (l_k - l_{k-1})$, we can write $p_{s,\infty}(l_1,...,l_s; \lambda) = \lambda \Omega(\lambda, l_1 - 1)\, s_0^{l_1} \prod_{k=2}^{s} [\lambda \Omega(\lambda, l_k - l_{k-1} - 1)\, s_0^{l_k - l_{k-1}}]$, which together with (i) gives (ii). By definition and Theorem A.1, $N(\lambda, M) = \lambda \partial \log \Omega(\lambda, M)/\partial \lambda \sim \lambda \partial \log[c_0(\lambda)\, s_0(\lambda)^{-M}]/\partial \lambda$, from which follows $\bar{p} = -\lambda s_0'(\lambda)/s_0(\lambda)$. But from $\lambda \varphi(s_0(\lambda)) = 1$ we immediately obtain $-\lambda s_0'(\lambda)/s_0(\lambda) = \varphi(s_0)/s_0 \varphi'(x_0)$ and hence (iii).

Theorem A.2. Let $N_M \in \mathbb{N}$ be any sequence with $\lim_{M \to \infty} N_M/M = \bar{p}$. Then

(i) $p_\infty(l) \equiv \lim_{M \to \infty} p(l; N_M, M) = p_\infty(l; \lambda) = \lambda \Omega(\lambda, l-1)\, s_0^l$

(ii) $\lim_{M \to \infty} p_s(l_1,..., l_s; N_M, M) = p_{s,\infty}(l_1,..., l_s; \lambda) = p_\infty(l_1; \lambda) \prod_{k=2}^{s} p_\infty(l_k - l_{k-1}; \lambda)$,

where $\lambda = 1/\varphi(s_0)$ and s_0 is the unique positive solution of $\varphi(s_0)/s_0 \varphi'(s_0) = \bar{p}$.

Proof. In order to derive the asymptotic limit of the occupation probability

$$p(l;N_M,M)=\sum_{r=1}^{l} Z(r-1,l-1)\,\frac{Z(N_M-r,M-l)}{Z(N_M,M)} \tag{A.7}$$

in the thermodynamic limit, we use (see Theorem 6.1 in ref. 26)

$$Z(N_M-1,M-1)=\frac{\varphi(s_M)^{N_M}}{\sigma_M s_M^M(2\pi N_M)^{1/2}}\,[1+\mathrm{O}(M^{-1})] \qquad \text{for} \quad M\to\infty \tag{A.8}$$

where $\sigma_M^2=\partial_u^2[\log\varphi(s_M e^u)]_{u=0}$ and s_M is the unique real positive solution of $N_M/M=\varphi(s)/s\varphi'(s)$.

We further define $\tilde{s}_M$ as the unique real positive root of $(N_M-r)/(M-l) =\varphi(s)/s\varphi'(s)$ (for r, l given integers) and $\tilde{\sigma}_M^2=\partial_u^2[\log\varphi(\tilde{s}_M e^u)]_{u=0}$. Then it is easy to show that there exist sequences β_M and γ_M converging to finite values for $M\to\infty$ with the property

$$\tilde{s}_M=s_M\left[1+\frac{\beta_M}{M}+\mathrm{O}(M^{-2})\right], \qquad \tilde{\sigma}_M=\sigma_M\left[1+\frac{\gamma_M}{M}+\mathrm{O}(M^{-2})\right] \tag{A.9}$$

(For example, $\beta_M=(l-r)\,f(s_M)/s_M f'(s_M)$ with $f(s)=\varphi(s)/s\varphi'(s)$ has the desired properties.) Replacing N_M by N_M-r, M by $M-l$, s_M by $\tilde{s}_M$, as well as σ_M by $\tilde{\sigma}_M$ in Eq. (A.8), and using Eq. (A.9), we obtain after simple calculations

$$\begin{aligned} &Z(N_M-r-1,M-l-1)\\ &\quad=Z(N_M-1,M-1)\,s_M^l\varphi(s_M)^{-r}\,[1+\mathrm{O}(M^{-1})] \qquad \text{for} \quad M\to\infty \end{aligned} \tag{A.10}$$

Taking the limit $M\to\infty$ in Eq. (A.7) we thus get (note that $\lim_{M\to\infty}s_M=s_0$)

$$\lim_{M\to\infty} p(l;N_M,M)=\sum_{r=1}^{l} Z(r-1,l-1)\,\varphi(s_0)^{-r}\,s_0^l=\lambda\Omega(\lambda,l-1)\,s_0^l \tag{A.11}$$

The proposition (ii) follows by using the asymptotic form of $Z(N_M-r,M-l)$ (Eq. (A.10) in formula (2.8)).

APPENDIX B

For $|s|<1$ and $\lambda \in (0, \infty)$ let

$$G(\lambda, s)=\frac{P(\lambda, s)}{Q(\lambda, s)}=\sum_{M=0}^{\infty} \Omega(\lambda, M)\, s^M=\frac{s^{2m-1}}{[1-s-\lambda s^{2m}]} \tag{B.1}$$

be the generating function from Eq. (2.11) for the special case of the hard rod interaction potential defined in Eq. (3.1).

Lemma B.1. The roots $s_0,..., s_{2m-1}$ of the polynomial $Q(\lambda, s)$ are all distinct.

Proof. For one of the roots s_i not to be simple, we must require that both $Q(\lambda, s_i)=0$ and $(\partial Q(\lambda, s)/\partial s)_{s=s_i}=0$. But if $(\partial Q(\lambda, s)/\partial s)_{s=s_i}=0$, we have $s_i^{2m-1}=-1/2m\lambda$ and inserting this result into $Q(\lambda, s_i)=0$ we obtain $s_i=2m/(2m-1)>0$, i.e., a positive real number. On the other hand, the only real solution of $s^{2m-1}=-1/2m\lambda$ is negative, which is a contradiction. Hence all roots must be simple.

Let

$$\begin{aligned} p_\infty(l, \lambda) &= \bar{p}+\sum_{j=1}^{2m-1} c_j(\lambda) \left(\frac{s_0}{|s_j|}\right)^l e^{-i\theta_j l} \\ &= \sum_{r=1}^{[l/2m]} \binom{l-1-(2m-1)\, r}{r-1} (1-s_0)^r\, s_0^{l-2mr} \end{aligned}$$

be the occupancy probability in the thermodynamic limit, where $[x]$ denotes the integer part of x (see Eq. (3.4), and Eqs. (2.14), (2.15), (3.3), and note that $\varphi(s_0)=s_0^{2m}/(1-s_0)$).

Lemma B.2. For $\lambda_\infty=1/\varphi(s_0)=(1-s_0)\, s_0^{-2m}$ with $s_0=(1-2m\bar{p})/[1-(2m-1)\,\bar{p}]$, $\bar{p}=N/M$ $(0<\bar{p}<1/2m)$, and $l^2/M^2=\mathrm{o}(M^{-1})$

(i) $p(l; N, M)=p_\infty(l; \lambda_\infty)[1+\mathrm{O}(l^2/M)]$

(ii) $p_s(l_1,..., l_s=l; N, M)=p_{s,\infty}(l_1,..., l_s=l; \lambda_\infty)[1+\mathrm{O}(l^2/M)]$

Proof. According to Eqs. (2.6),

$$p(l; N, M)=\sum_{r=1}^{N} Z(r-1, l-1)\, \frac{Z(N-r, M-l)}{Z(N, M)} \tag{B.2}$$

With the definition

$$f(x, y) \equiv \log \binom{\nu M + x}{\bar{p} M + y} \tag{B.3}$$

where $\nu = 1 - (2m-1)\,\bar{p}$, and x, y are integers, we can write (see the results for $Z(N, M)$ in Eq. (3.3))

$$\frac{Z(N-r, M-l)}{Z(N, M)} = \exp[f((2m-1)(r-1) - l, -r) - f(-(2m-1), 0)] \tag{B.4}$$

If $x, y = O(l)$ we obtain, by applying Stirling's formula, $n! = (2\pi n)^{1/2}\,(n/e)^n \exp[O(1/n)]$,

$$f(x, y) = \frac{1}{2} \log\left(\frac{\nu}{2\pi\bar{p}(\nu - \bar{p})\,M}\right) + M[\nu \log \nu - (\nu - \bar{p}) \log(\nu - \bar{p}) - \bar{p} \log \bar{p}]$$
$$+ x \log \nu - (x - y) \log(\nu - \bar{p}) - y \log \bar{p} + O\left(\frac{l^2}{M}\right) \tag{B.5}$$

Note that the sum over r in Eq. (B.2) runs at most up to the integer part of $l/2m$, such that the arguments of the f functions appearing in Eq. (B.4) are all of order $O(l)$. Accordingly,

$$\frac{Z(N-r, M-l)}{Z(N, M)} = (1 - s_0)^r\, s_0^{(l-2mr)}[1 + O(l^2/M)] \tag{B.6}$$

from which we obtain (i) by using Eq. (B.2).

Analogously, starting with Eq. (2.8),

$$p_s(l_1, ..., l_s; N, M) = \sum_{1 \leqslant r_1 < \cdots < r_s \leqslant N} Z(r_1 - 1, l_1 - 1)$$
$$\times \prod_{k=1}^{s-1} Z(r_{k+1} - r_k - 1, l_{k+1} - l_k - 1)\,\frac{Z(N - r_s, M - l_s)}{Z(N, M)} \tag{B.7}$$

and again using Eq. (B.6) for the asymptotic behavior, we obtain (ii) after straightforward algebra.

Lemma B.3. Let λ be the unique fugacity corresponding to given mean number density $\bar{p} \in (0, 1/2m)$, and $\lambda_\infty = 1/\varphi(s_0) = (1-s_0)\, s_0^{-2m}$ with $s_0 = (1-2m\bar{p})/[1-(2m-1)\,\bar{p}]$. Then for $l/M = \mathrm{o}(1)$,

(i) $\tilde{p}(l; \lambda, M) = p_\infty(l; \lambda_\infty)[1 + \mathrm{O}(l/M)]$

(ii) $\tilde{p}_s(l_1,..., l_s = l; \lambda, M) = p_{s,\infty}(l_1,..., l_s = l; \lambda_\infty)[1 + \mathrm{O}(l/M)]$

Proof. According to Eq. (2.10)

$$\tilde{p}(l; \lambda, M) = \lambda\Omega(\lambda, l-1)\,\frac{\Omega(\lambda, M-l)}{\Omega(\lambda, M)} \tag{B.8}$$

where $\Omega(\lambda, M) = \sum_{j=0}^{2m-1} c_j(\lambda)\, s_j(\lambda)^{-M}$ (see Lemma B.1 and the discussion after Eq. (2.11)). In order to find the asymptotic behavior for $M \to \infty$, one has to keep in mind that λ depends on M. Let us denote by λ_M the fugacity corresponding to the mean number density $\bar{p}$ in a system of (finite) size M, i.e., the unique solution of $\bar{p} = \lambda M^{-1}\,\partial \log \Omega(\lambda, M)/\partial\lambda$ (see Corollary A.1). In leading order λ_M approaches λ_∞ as

$$\lambda_M = \lambda_\infty \left[\,1 + \frac{b}{M} + \mathrm{O}\left(\frac{1}{M^2}\right)\right] \tag{B.9}$$

where b is a constant independent of M. The proof of this relation can be worked out by writing $\lambda_M = \lambda_\infty + \varepsilon_M$ with $\lim_{M\to\infty} \varepsilon_M = 0$,[4] and inserting this into the determining equation for λ_M. Careful expansion of the coefficients $c_j(\lambda_M)$ and the powers $s_j(\lambda_M)^{-M}$ with respect to ε_M in the expression for $\Omega(\lambda_M, M)$ then yields $\lim_{M\to\infty} \varepsilon_M M = b\lambda_\infty$ and $\lim_{M\to\infty} [\varepsilon_M - b\lambda_\infty/M]\, M^2 = \text{const.}$

Using Eq. (B.9) we find

$$\Omega(\lambda_M, M-l) = \exp(b\bar{p})\, c_0(\lambda_\infty)\, s_0(\lambda_\infty)^{-(M-l)} \left[\,1 + \mathrm{O}\left(\frac{l}{M}\right)\right] \tag{B.10}$$

and thus obtain $\Omega(\lambda, M-l)/\Omega(\lambda, M) = s_0(\lambda_\infty)^l\,[1 + \mathrm{O}(l/M)]$. Since $\lambda_M\Omega(\lambda_M, l-1) = \lambda_\infty\Omega(\lambda_\infty, l-1)[1 + \mathrm{O}(l/M)]$, it follows (i) from Eq. (B.8). Analogously, (ii) follows by using Eq. (2.9) and the asymptotic expansion (B.10).

[4] Note that, according to Corollary A.1 we have for $\lambda_\infty = 1/\varphi(s_0)$, $\lim_{M\to\infty} N(\lambda_\infty, M)/M = \bar{p}$, i.e. because of the one-to-one correspondence between $\bar{p}$ and λ it must hold $\lim_{M\to\infty} \lambda_M = \lambda_\infty$.

Theorem B.1. If $(M-1)-(4m-2)\,N>0$ then the occupation probability $p(l; N, M)$ is independent of l for all $l \in \mathscr{R}_1 \equiv \{l \in \mathbb{N} \mid l^{(1)} \leqslant l \leqslant M+1-l^{(1)}\}$, with $l^{(1)} \equiv (2m-1)\,N+1$, i.e. we can write $p(l; N, M) = \bar{u}(N, M)/Z(N, M)$. At the outer boundary points $l^{(-)} \equiv l^{(1)}-1$ and $l^{(+)} \equiv M+2-l^{(1)}$, $p(l^{(\mp)}; N, M)$ is different from $p(l; N, M)$ inside $\mathscr{R}_1$, in particular $p(l^{(\mp)}; N, M) = [\bar{u}(N, M) + (-1)^N]/Z(N, M)$.

Proof. Given $p(l; N, M)$ from Eq. (2.6) we first show that

$$\begin{aligned} u(l; N, M) &\equiv \sum_{r=1}^{N} Z(r-1, l-1)\, Z(n-r, M-l) \\ Z(r, l) &= \binom{l-(2m-1)(r+1)}{r} \end{aligned} \tag{B.11}$$

is constant inside $\mathscr{R}_1$ as long as $(M-1)-(4m-2)\,N>0$. To this end we will proof that $u(l; N, M)$ for $l \in \mathscr{R}_1$ can be rewritten by use of the following combinatorial identity

$$\begin{aligned} u(l; N, M) &= \sum_{r=1}^{N} \binom{l-1-(2m-1)\,r}{r-1} \binom{M-l-(2m-1)(N+1-r)}{N-r} \\ &= \binom{M+1-4m-(2m-1)(N-1)}{N-1} \\ &\quad - \sum_{r=2}^{N} (-1)^r \binom{2m(r-1)-1}{r-1} \binom{M+1-4m-(2m-1)(N-r)}{N-r} \\ &\equiv \bar{u}(N, M) \end{aligned} \tag{B.12}$$

which is independent of l.

To verify the combinatorial formula we follow the methods described in the book of Riordan on combinatorial identities[27] and use the following theorem of Lagrange for implicit functions:[28] Let $\phi(z)$ be a power series in z with $\phi(0) \neq 0$, and let $z(t)$ be the unique power series with $z(0)=0$ satisfying the implicit equation $z(t) = t\phi(z(t))$. Then, for any power series $F(z)$,

$$\frac{F(z)}{(1-t\Phi'(z))} = \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{d^n}{d\lambda^n} \{F(\lambda)\, \Phi(\lambda)^n\} \,|_{\lambda=0} \tag{B.13}$$

Applying this theorem to $\phi(z) = (1+z)^{-\beta}$ and $F(z) = (1+z)^{\alpha}$ with $|z|<1$ and $\alpha, \beta \in \mathbb{N}$ one obtains

$$\frac{(1+z)^{\alpha+1}}{1+(\beta+1)\,z}=\sum_{n=0}^{\infty}\omega(\alpha,n)\,t^n$$

$$\omega(\alpha,n)=\begin{cases}\binom{\alpha-\beta n}{n}, & 0\leqslant n\leqslant\frac{\alpha}{\beta}\\ (-)^n\binom{(\beta+1)\,n-\alpha-1}{n}, & n>\frac{\alpha}{\beta}\end{cases}\tag{B.14}$$

Using (B.14) we can write

$$\begin{aligned}\frac{(1+z)^{\alpha+\gamma+2}}{[1+(\beta+1)\,z]^2}&=\left[\frac{(1+z)}{1+(\beta+1)\,z}\right]\left[\frac{(1+z)^{\alpha+\gamma+1}}{1+(\beta+1)\,z}\right]\\ &=\sum_{n=0}^{\infty}\omega(0,n)\,t^n\sum_{n=0}^{\infty}\omega(\alpha+\gamma,n)\,t^n\end{aligned}\tag{B.15}$$

and

$$\begin{aligned}\frac{(1+z)^{\alpha+\gamma+2}}{[1+(\beta+1)\,z]^2}&=\left[\frac{(1+z)^{\alpha+1}}{1+(\beta+1)\,z}\right]\left[\frac{(1+z)^{\gamma+1}}{1+(\beta+1)\,z}\right]\\ &=\sum_{n=0}^{\infty}\omega(\alpha,n)\,t^n\sum_{n=0}^{\infty}\omega(\gamma,n)\,t^n\end{aligned}\tag{B.16}$$

Comparing (B.15) with (B.16) and equating expansion coefficients we obtain

$$\sum_{k=0}^{n}\omega(0,k)\,\omega(\alpha+\gamma,n-k)=\sum_{k=0}^{n}\omega(\alpha,k)\,\omega(\gamma,n-k)\tag{B.17}$$

In particular, for $n\leqslant\min\{[\alpha/\beta];[\gamma/\beta]\}$ (see Eq. (B.14)),[5]

$$\begin{aligned}&\sum_{k=0}^{n}\binom{\alpha-\beta k}{k}\binom{\gamma-\beta(n-k)}{n-k}\\ &\quad=\binom{\alpha+\gamma-\beta n}{n}+\sum_{k=1}^{n}(-1)^k\binom{(\beta+1)\,k-1}{k}\binom{\alpha+\gamma-\beta(n-k)}{n-k}\end{aligned}\tag{B.18}$$

By setting $n=N-1$, $k=r-1$, $\beta=2m-1$, $\alpha=l-2m$, and $\gamma=M+1-2m-l$ for $l\in\mathscr{R}_1$ (i.e., for $(2m-1)\,N+1\leqslant l\leqslant M-(2m-1)\,N$), we have

[5] Equation (B.18) may be identified as a combinatorial identity derived explicitly in the book of Riordan on p. 148[(27)] by replacing β by $-\beta$. However, in order to do this one has to define the binomial coefficients for negative entries by analytical continuations of the Gamma function.

$N-1 \leqslant \min\{[(l-2m)/(2m-1)], [(M+1-2m-l)/(2m-1)]\}$, and can use Eq. (B.18) to get Eq. (B.12).

In order to show that $\mathscr{R}_1$ is a "maximal" set, we again use Eq. (B.17) with $\alpha = l^{(\mp)} - 2m$, $\beta = 2m-1$, $\gamma = M+1-2m-l^{(\mp)}$, $n = N-1$ and $r = k-1$ (note that due to symmetry, we can restrict ourselves to $\alpha = l^{(-)} - 2m$ and $\gamma = M+1-2m-l^{(-)}$, so that $n-1 \leqslant \alpha/\beta$, $n > \alpha/\beta$, $n \leqslant \gamma/\beta$ with $\omega(\gamma, 0) = 1$ and $\omega(\alpha/n) = (-1)^n$) to obtain

$$u(l^{(\mp)}; N, M) = \bar{u}(N, M) + (-1)^N \tag{B.19}$$

This completes the proof of theorem B.1.

Corollary B.1. For $M+1 \geqslant 6m$ (that means there can be more than just one rod in the system) there does not exist a central region where $\tilde{p}(l; \lambda, M)$ is constant (except for the trivial set $\tilde{\mathscr{R}}_1 = \{M/2, M/2+1\}$ for even M).

Proof. Assume that there exist a non-trivial central region $\tilde{\mathscr{R}}_1 = \{l_0, ..., M+1-l_0\}$ with $2m \leqslant l_0 \leqslant (M-1)/2$ in which $\tilde{p}(l; \lambda, M)$ is constant. Then there exists a function

$$f(\lambda, M) = \lambda \Omega(\lambda, l-1)\, \Omega(\lambda, M-l) \tag{B.20}$$

independent of l for all $l \in \tilde{\mathscr{R}}_1$.

From

$$\lambda \Omega(\lambda, l-1)\, \Omega(\lambda, M-l) = \sum_{N=1}^{N_0} Z(N, M)\, p(l, N, M)\, \lambda^N \tag{B.21}$$

for $N_0 = \max\{N \geqslant 1; Z(N, M) > 0\} = [(M+1)/2m] - 1$ (note that $Z(N, M) = \binom{M-(2m-1)(N+1)}{N}$), we get

$$p(l, N, M) = \frac{1}{Z(N, M)\, N!} \left. \frac{\partial^N f(\lambda, M)}{\partial^N \lambda} \right|_{\lambda=0} = \text{const} \tag{B.22}$$

for all $l \in \tilde{\mathscr{R}}_1$ and all $1 \leqslant N \leqslant N_0$. But, according to Theorem B.1, we have $p(l, N, M) = \text{const}$ in a central region if and only if $l \in \mathscr{R}_1$. Therefore,

$$\tilde{\mathscr{R}}_1 \subseteq \mathscr{R}_1 = \{(2m-1)\, N+1, ..., M-(2m-1)\, N\} \qquad \text{for} \quad 1 \leqslant N \leqslant N_0 \tag{B.23}$$

Choosing $N = N_0$ (and because we require $\tilde{\mathscr{R}}_1$ to have more than two elements for excluding trivial situations), we obtain

$$(2m-1)\, N_0 + 4 \leqslant M+1-(2m-1)\, N_0 \tag{B.24}$$

from which one readily concludes that $M+1 \leqslant 6m-1$ in contradiction to the restriction imposed on M.

Comment. One can even show[18] that there does not exist *any* non-trivial region inside which $\tilde{p}(l; \lambda, M)$ is constant.

Theorem B.2. If $M-1-(4m-2)N+2(m-1)(s-1)>0$ then the joint probabilities $p_s(l_1,..., l_s; N, M)$ are translationally invariant for $(l_1,..., l_s) \in \mathcal{R}_s = \{(l_1,..., l_s) \in \mathbb{N}^s \mid l^{(s)} \leqslant l_1;\ 2m \leqslant l_k - l_{k-1}$ for $k=2,..., s;\ l_s \leqslant M+1-l^{(s)}\}$ with $l^{(s)} \equiv (2m-1)(N+1-s)+1$, i.e., there exists a function $f(y_1,..., y_{s-1}; N, M)$ exhibiting the property

$$p_s(l_1,..., l_s; N, M) = f(l_2-l_1,..., l_s-l_{s-1}; N, M) \tag{B.25}$$

If $(l_1,..., l_s) \notin \mathcal{R}_s$ and $(l_1,..., l_r \pm 1,..., l_s) \in \mathcal{R}_s$ for some $\tau \in \{1,..., s\}$ then

$$p_s(l_1,..., l_s; N, M) = f(l_2-l_1,..., l_s-l_{s-1}; N, M) + (-1)^{N+1-s}/Z(N, M) \tag{B.26}$$

Proof. The joint probabilities $p(l_1,..., l_s; N, M)$ are given by (see Eq. (2.8))

$$p_s(l_1,..., l_s; N, M) = \sum_{1 \leqslant r_1 < \cdots < r_s \leqslant N} \frac{Z(r_1-1, l_1-1)\, Z(N-r_s, M-l_s)}{Z(N, M)} \times \prod_{k=2}^{s} Z(r_k - r_{k-1} - 1, l_k - l_{k-1} - 1) \tag{B.27}$$

By introducing new variables $x_1 = r_1$, $x_k = r_k - r_{k-1}$ for $k=2,..., s$ $(\sum_{k=1}^{s} x_k = r_s)$ we can rewrite this as

$$\begin{aligned} p_s(l_1,..., l_s; N, M) &= \sum_{(x_1,..., x_s) \in \mathcal{A}_{N, s}} \frac{Z(x_1-1, l_1-1)\, Z(N-\sum_{i=1}^{s} x_i, M-l_s)}{Z(N, M)} \times \prod_{k=2}^{s} Z(x_k-1, l_k-l_{k-1}-1) \\ &= Z(N, M)^{-1} \sum_{(x_2,..., x_s) \in \mathcal{A}_{N-1, s-1}} \left\{ \prod_{k=2}^{s} Z(x_k-1, l_k-l_{k-1}-1) \right. \\ &\quad \left. \times \sum_{x_1=1}^{N-\sum_{i=2}^{s} x_i} Z(x_1-1, l_1-1)\, Z\left(N - \sum_{i=2}^{s} x_i - x_1, M-l_s\right) \right\} \end{aligned} \tag{B.28}$$

where $\mathcal{A}_{N, s} \equiv \{(x_1,..., x_s) \in \mathbb{N}^s \mid x_1 + \cdots + x_s \leqslant N\}$.

Setting $N' = N - \sum_{i=2}^{s} x_i$ and $M' = M - (l_s - l_1)$, we have from Theorem B.1 (see Eq. (B.11))

$$\sum_{x_1=1}^{N'} Z(x_1 - 1, l_1 - 1)\, Z(N' - x_1, M' - l_1) = u(l_1; N', M') \tag{B.29}$$

where $u(l_1; N', M') = \bar{u}(N', M') = \text{const}$ for $(2m-1)\, N' + 1 \leqslant l_1 \leqslant M' - (2m-1)\, N'$. For the x_i this means $(2m-1)(N - \sum_{i=2}^{s} x_i) + 1 \leqslant l_1 \leqslant M - (l_s - l_1) - (2m-1)(N - \sum_{i=2}^{s} x_i)$. The latter inequality holds true for all $(x_2,..., x_s) \in \mathscr{A}_{N-1, s-1}$, if $(2m-1)(N+1-s) + 1 \leqslant l_1$ and $l_s \leqslant M - (2m-1)(N+1-s)$, i.e., for $(l_1,..., l_s) \in \mathscr{R}_s$. Since $(l_s - l_1) = \sum_{k=2}^{s} (l_k - l_{k-1})$ we obtain

$$\begin{aligned} p(l_1,..., l_s; N, M) &= \sum_{(x_2,..., x_s) \in \mathscr{A}_{N-1, s-1}} \prod_{k=2}^{s} Z(x_k - 1, l_k - l_{k-1} - 1) \\ &\quad \times \frac{\bar{u}(N - \sum_{i=2}^{s} x_i, M - \sum_{i=2}^{s} (l_i - l_{i-1}))}{Z(N, M)} \\ &\equiv f(l_2 - l_1,..., l_s - l_{s-1}; N, M) \end{aligned} \tag{B.30}$$

which completes the proof of the first part of the theorem.

To prove the second part, we insert Eq. (B.29) in Eq. (B.28) and consider an outer boundary point with $(l_1,..., l_s) \notin \mathscr{R}_s$ and $(l_1,..., l_\tau \pm 1,..., l_s) \in \mathscr{R}_s$ for some $\tau \in \{1,..., s\}$. In fact, according to the constraints implied by the finite rod lengths, one can show that only $\tau = 1$ and $\tau = s$ are possible. Due to symmetry we can restrict ourselves to the case $\tau = 1$. Then the outer boundary point is $(l_1 = l^{(s)} - 1, l_2,..., l_s)$ and we obtain

$$\begin{aligned} &p_s(l_1 = l^{(s)} - 1,..., l_s; N, M) \\ &\quad = \frac{1}{Z(N, M)} \sum_{\mathscr{A}_{N-1, s-1}} \left\{ \prod_{k=2}^{s} Z(x_k - 1, l_k - l_{k-1} - 1)\, u(l_1; N', M') \right\}_{l_1 = l^{(s)} - 1} \end{aligned} \tag{B.31}$$

Except for the particular configuration $(x_2 = 1,..., x_s = 1)$, all configurations $(x_2,..., x_s) \in \mathscr{A}_{N-1, s-1}$ yield arguments (l_1, N', M') for which $u(l_1, N', M')$ is constant (see the discussion above). For $(x_2 = 1,..., x_s = 1)$, l_1 is an outer boundary point of the set $\mathscr{R}_1$ corresponding to a system of size M' with N'

rods. According to Theorem B.1 we thus have $u(l_1, N', M') = \bar{u}(N', M') + (-1)^{N'}$. By inserting these results in Eq. (B.31) and by using the definition of $f(y_1,..., y_{s-1}; N, M)$ in Eq. (B.30) we obtain

$$p_s(l_1 = l^{(s)} - 1,..., l_s; N, M) = f(l_2 - l^{(s)} + 1,..., l_s - l_{s-1}; N, M) + \frac{(-1)^{N+1-s}}{Z(N, M)} \tag{B.32}$$

Corollary B.2. For $(l_1,..., l_s) \notin \mathscr{C}_s \equiv \{(l_1,..., l_s) \in \mathbb{N}^s \mid 2m \leqslant l_1 < 4m, 2m \leqslant l_k - l_{k-1}$ for $k = 1,..., s$; $M + 1 - 4m < l_s \leqslant M + 1 - 2m\}$ (see footnote 1 in Section 3.2) there does not exist a region, where $\tilde{p}_s(l_1,..., l_s; \lambda, M)$ is translationally invariant.

Proof. If $\tilde{p}_s(l_1,..., l_s; \lambda, M) = \tilde{f}(l_2 - l_1,..., l_s - l_{s-1}; \lambda, M)$ for some $(l_1,..., l_s) \notin \mathscr{C}_s$ then, from Eq. (2.9),

$$\Omega(\lambda, l_1 - 1)\, \Omega(\lambda, M' - l_1) = \frac{\Omega(\lambda, M)}{\lambda^s}\, \tilde{f}(l_2 - l_1,..., l_s - l_{s-1}; \lambda, M) \times \prod_{k=2}^{s} \frac{1}{\Omega(\lambda, l_k - l_{k-1} - 1)} \tag{B.33}$$

where $M' = M - (l_s - l_1)$. Accordingly, there exists a range of consecutive l_1 values, where $\Omega(\lambda, l_1 - 1)\, \Omega(\lambda, M' - l_1)$ is independent of l_1. This, however, is impossible due to the comment after Corollary B.1.

Theorem B.3. If $M - 2(2m-1)(N+1-s) \geqslant 0$ then the joint probabilities $p_s(l_1,..., l_s; N, M)$ are constant functions for $(l_1,..., l_s) \in \mathscr{B}_s \equiv \{(l_1,..., l_s) \in \mathbb{N}^s \mid (2m-1)(N+1-s) + 2 \leqslant l_1;\ (2m-1)(N+1-s) + 1 \leqslant l_k - l_{k-1}$ for $k = 2,..., s$; $l_s \leqslant M - (2m-1)(N+1-s)\}$, i.e., we can write $p_s(l_1,..., l_s; N, M) = \bar{v}(N, M)$. If $(l_1,..., l_s) \notin \mathscr{B}_s$ and $(l_1,..., l_\tau \pm 1,..., l_s) \in \mathscr{B}_s$ for some $\tau \in \{1,..., s\}$ then

$$p_s(l_1,..., l_s; N, M) = \bar{v}(N, M) + \frac{(-1)^{N+1-s}}{Z(N, M)} \tag{B.34}$$

Proof. The explicit formula (see Eqs. (2.8), (3.3)

$$Z(N, M)\, p_s(l_1,..., l_s; N, M) = \sum_{(x_1,..., x_s) \in \mathscr{A}_{N,s}} \binom{l_1 - 1 - (2m-1)\, x_1}{x_1 - 1}$$

$$\times \binom{M+1-2m-l_s-(2m-1)\left(N-\sum_{i=1}^{s} x_i\right)}{N-s-\sum_{i=1}^{s} x_i}$$
$$\times \prod_{k=2}^{s} \binom{l_k-l_{k-1}-1-(2m-1)(x_k-x_{k-1})}{x_k-x_{k-1}-1} \tag{B.35}$$

can be rewritten by using Eq. (B.14) derived in Theorem B.1 (remember that we defined $\mathscr{A}_{N,s}=\{(x_1,..., x_s)\in \mathbb{N}^s) \mid x_1+\cdots+x_s\leqslant N\}$ after Eq. (B.28)). We have for $\alpha_i\geqslant 0$, $i=1,..., s+1$, and $\mathscr{E}_{n,s}\equiv\{(n_1,..., n_s)\in \mathbb{N}_0^s \mid n_1+\cdots+n_s=n\}$,

$$\frac{(1+z)^{\alpha_1+\cdots+\alpha_{s+1}+s+1}}{[1+(\beta+1)z]^{s+1}}=\prod_{k=1}^{s+1}\sum_{n_k=0}^{\infty}\omega(\alpha_k,n_k)\,t^{n_k}$$
$$=\sum_{n=0}^{\infty}t^n\sum_{(n_1,...,n_{s+1})\in\mathscr{E}_{n,s+1}}\prod_{k=1}^{s+1}\omega(\alpha_k,n_k) \tag{B.36}$$

and

$$\frac{(1+z)^{\alpha_1+\cdots+\alpha_{s+1}+1}(1+z)^s}{[1+(\beta+1)z]^1[1+(\beta+1)z]^s}$$
$$=\prod_{n_1=0}^{\infty}\omega(\alpha_1+\cdots+\alpha_{s+1},n_1)\,t^{n_1}\prod_{k=2}^{s+1}\sum_{n_k=0}^{\infty}\omega(0,n_k)\,t^{n_k}$$
$$=\sum_{n=0}^{\infty}t^n\sum_{\mathscr{E}_{n,s+1}}\omega(\alpha_1+\cdots+\alpha_{s+1},n_1)\prod_{k=2}^{s+1}\omega(0,n_k) \tag{B.37}$$

Comparing (B.36) and (B.37) and equating coefficients we obtain

$$\sum_{(n_1,...,n_{s+1})\in\mathscr{E}_{n,s+1}}\prod_{k=1}^{s+1}\omega(\alpha_k,n_k)$$
$$=\sum_{(n_1,...,n_{s+1})\in\mathscr{E}_{n,s+1}}\omega(\alpha_1+\cdots+\alpha_{s+1},n_1)\prod_{k=2}^{s+1}\omega(0,n_k) \tag{B.38}$$

which, for $n\leqslant\min_{1\leqslant k\leqslant s+1}\{[\alpha_k/\beta]\}$ (see Eq. (B.14)), yields

$$\sum_{\mathscr{E}_{n,s+1}}\prod_{k=1}^{s+1}\binom{\alpha_k-\beta n_k}{n_k}$$
$$=\sum_{\mathscr{E}_{n,s+1}}\binom{\alpha_1+\cdots+\alpha_{s+1}-\beta n_1}{n_1}\prod_{k=2}^{s+1}(-1)^{n_k}\binom{(\beta+1)\,n_k-1}{n_k} \tag{B.39}$$

We have defined $\binom{-1}{0}=1$ on the right side here (but not on the left hand side).

By choosing $\alpha_1=l_1-2m$, $\alpha_k=l_k-l_{k-1}-2m$ for $k=2,..., s$, $\alpha_{s+1}=M+1-l_s-2m$, $\beta=2m-1$ and $n=N-s\leqslant \min_{1\leqslant k\leqslant s+1}\{\alpha_k/\beta\}$ (for all $(l_1, ..., l_s)\in \mathscr{B}_s$), we can identify the combinatorial expression (B.36) by the left hand side of (B.39). Substituting the right hand side we then obtain

$$\begin{aligned}
p_s(l_1,..., l_s; N, M) &= Z(N, M)^{-1} \sum_{(x_1,..., x_s)\in \mathscr{A}_{N,s}} (-1)^{N-\sum_{i=<1}^{s} x_i} \\
&\quad \times \binom{2m\left(N-\sum_{i=1}^{s} x_i\right)-1}{N-\sum_{i=1}^{s} x_i} \binom{M-2ms-(2m-1)\,x_1}{x_1-1} \\
&\quad \times \prod_{k=2}^{s} (-1)^{x_k-1} \binom{2m(x_k-1)-1}{x_k-1} \\
&\equiv \bar{v}(N, M)
\end{aligned} \tag{B.40}$$

which completes the proof of the first part of the theorem.

Now, let $(l_1,..., l_s)\notin \mathscr{B}_s$ and $(l_1,..., l_\tau\pm 1,..., l_s)\in \mathscr{B}_s$ for a given $\tau\in\{1,..., s\}$, and $l_0=0$ and $l_{s+1}=M+1$. Then $N-s\leqslant [\alpha_k/(2m-1)]$ for $k\neq\tau$ and $N-s-1=[\alpha_\tau/(2m-1)]$, which can be shown by simple topological considerations. Accordingly, for $(n_1,..., n_{s+1})\in \mathscr{E}'_{N-s,\, s+1}\equiv \mathscr{E}_{N-s,\, s+1}\backslash(n_1=0,..., n_\tau=N-s,..., n_{s+1}=0)$, $\omega(\alpha_k, n_k)=\binom{\alpha_k-(2m-1)\,n_k}{n_k}$, while for the particular element $(n_1=0,..., n_\tau=N-s,..., n_{s+1}=0)$, $\omega(\alpha_k, n_k)=(1-\delta_{k\tau})+(-1)^{(N-s)}\,\delta_{k\tau}$. Evaluating the left hand side of Eq. (B.38) we arrive at

$$\begin{aligned}
&\sum_{(n_1,..., n_{s+1})\in \mathscr{E}_{N-s,\, s+1}} \prod_{k=1}^{s+1} \omega(\alpha_k, n_k) \\
&\quad = \sum_{(n_1,..., n_{s+1})\in \mathscr{E}'_{N-s,\, s+1}} \prod_{k=1}^{s+1} \binom{\alpha_k-(2m-1)\,n_k}{n_k} + (-1)^{N-s} \\
&\quad = Z(N, M)\, p_s(l_1,..., l_s; N, M) + (-1)^{N-s}
\end{aligned} \tag{B.41}$$

On the other hand, the right hand side of Eq. (B.38) is equal to $Z(N, M)\,\bar{v}(N, M)$ and hence we obtain

$$p_s(l_1,..., l_s; N, M)=\bar{v}(N, M)+\frac{(-1)^{N+1-s}}{Z(N, M)} \tag{B.42}$$

APPENDIX C

For $0 \leqslant M' + \alpha \leqslant M$ and $\alpha \geqslant 0$, $\Omega(\lambda; M', \alpha)$ is defined as follows (for $v(n) = v_{\mathrm{HR}}(n)$, see Section 3)

$$
\begin{aligned}
&\Omega(\lambda; M', \alpha) = 0, \qquad \text{for} \quad M' < 2m - 1 \\
&\Omega(\lambda; M', \alpha) = 1, \qquad \text{for} \quad 2m - 1 \leqslant M' < 4m - 1 \\
&\Omega(\lambda; M', \alpha) = 1 + \lambda \sum_{r=2m}^{M'+1-2m} e^{-u(\alpha + r)} \Omega(\lambda, r-1, \alpha), \qquad \text{for} \quad M' \geqslant 4m - 1
\end{aligned}
\tag{C.1}
$$

Theorem C.1. The occupation probability

$$
\tilde{p}(l; \lambda, M) = \lambda e^{-u(l)} \frac{\Omega(\lambda; l-1, 0)\, \Omega(\lambda; M-l, l)}{\Omega(\lambda; M, 0)}
\tag{C.2}
$$

is the unique solution of the following set of nonlinear coupled difference equations

$$
\begin{aligned}
0 = -\log \lambda + u(l) + \log \tilde{p}_l + \sum_{s=l+1}^{l+2m-1} \log[1 - t_m(s) + \tilde{p}_s] \\
- \sum_{s=l}^{l+2m-1} \log[1 - t_m(s)]
\end{aligned}
\tag{C.3}
$$

for $l \in \{2m, ..., M+1-2m\}$ and $\tilde{p}_l = 0$ else, where $t_m(s) = \sum_{j=0}^{2m-1} \tilde{p}_{s-j}$.

Lemma C.1. Let $M' \geqslant 2m$. If $0 \leqslant M' + \alpha \leqslant M$ and $\alpha \geqslant 0$, then $\Omega(\lambda; M', \alpha)$ obeys the recursion relations.

(i) $\Omega(\lambda, M', \alpha) = \Omega(\lambda; M'-1, \alpha) + \lambda^{-u(\alpha + M' - 2m + 1)} \Omega(\lambda; M' - 2m, \alpha)$,

(ii) $\Omega(\lambda, M', \alpha) = \Omega(\lambda; M'-1, \alpha+1) + \lambda e^{-u(\alpha + 2m)} \Omega(\lambda; M' - 2m, \alpha + 2m)$,

Lemma C.2. For $s \geqslant 2m$ let

$$
1 - t_m(s) = \frac{\Omega(\lambda; s-1, 0)}{\Omega(\lambda; M, 0)} \phi(\lambda; M, s)
\tag{C.4}
$$

Then $\phi(\lambda; M, s)$ obeys for $\tilde{p}_s \equiv \tilde{p}(s; \lambda, M)$ (from Eq. (C.2)) the relations

(i) $\phi(\lambda; M, s) = \Omega(\lambda; M - s + 2m - 1, s - 2m + 1)$,

(ii) $\phi(\lambda; M, s-1) = \phi(\lambda; M, s) + \lambda e^{-u(s)} \Omega(\lambda; M - s, s)$.

Proof of Lemma C.1. For $M' \geqslant 4m-1$

$$\Omega(\lambda; M', \alpha) = 1 + \lambda \sum_{r=2m}^{M'-2m} e^{-u(\alpha+r)} \Omega(\lambda; r-1, \alpha) + \lambda e^{-u(\alpha+M'-2m+1)} \Omega(\lambda; M'-2m, \alpha)$$

$$= \Omega(\lambda; M'-1, \alpha) + e^{-u(\alpha+M'-2m+1)} \Omega(\lambda; M'-2m, \alpha) \tag{C.5}$$

If $2m \leqslant M' < 4m-1$, then $\Omega(\lambda; M'-1, \alpha) = 1$ and $\Omega(\alpha; M'-2m, \alpha) = 0$. Hence, Eq. (C.5) is also valid for $2m \leqslant M' < 4m-1$, which implies (i).

According to (2.2),

$$Z(N, M', \alpha) = \sum_{1 \leqslant i_1, \dots < i_N \leqslant M'} \exp -\left[\sum_{k=1}^{N} u(\alpha + i_k) + v(i_1) + \sum_{k=2}^{N} v(i_k - i_{k-1}) + v(M'+1-i_N) \right]$$

$$= \sum_{l=1}^{M'} e^{-u(\alpha+l)-v(l)} \times \sum_{l+1 \leqslant i_2, \dots < i_N \leqslant M'} \exp -\left[\sum_{k=2}^{N} u(\alpha+i_k) + v(i_2 - l) + \sum_{k=3}^{N} v(i_k - i_{k-1}) + v(M'+1-i_N) \right]$$

$$= \sum_{l=1}^{M'} \exp -[u(\alpha+l) + v(l)] \times \sum_{1 \leqslant j_1 < \cdots < j_{N-1} \leqslant M'-l} \exp -\left[\sum_{k=1}^{N-1} u(\alpha+l+j_k) + v(j_1) + \sum_{k=2}^{N-1} v(j_k - j_{k-1}) + v(M'-l+1-j_{N-1}) \right]$$

$$= \sum_{l=1}^{M'} e^{-u(\alpha+l)} e^{-v(l)} Z(N-1, M'-l, \alpha+l) \tag{C.6}$$

Remembering that $Z(0, M', \alpha) = e^{-v(M'+1)}$ (see the remark right after Eq. (2.3)), it holds

$$\Omega(\lambda, M', \alpha) = \sum_{N=0}^{\infty} Z(N, M', \alpha)\, \lambda^N$$
$$= e^{-v(M'+1)} + \lambda \sum_{l=1}^{M'} e^{-u(\alpha+l)} e^{-v(l)}\, \Omega(\lambda, M'-l, \alpha+l) \qquad \text{(C.7)}$$

where $v(n) = \infty$ for $n < 2m$, and $v(n) = 0$ for $n \geqslant 2m$. Since $\Omega(\lambda, M'-l, \alpha+l) = 0$ for $M'-l < 2m-1$ we have

$$\Omega(\lambda, M', \alpha) = 1 + \lambda \sum_{l=2m}^{M'} e^{-u(\alpha+l)} \Omega(\lambda, M'-l, \alpha+l) \qquad \text{(C.8)}$$

which for $r = M' - l$ yields

$$= 1 + \lambda \sum_{r=2m-1}^{M'-1-2m} e^{-u(\alpha+M'-r)} \Omega(\lambda; r, \alpha+M'-r) \qquad \text{(C.9)}$$

Hence we finally obtain (ii),

$$\Omega(\lambda, M', \alpha) = 1 + \lambda \sum_{r=2m-1}^{M'-2m} e^{-u(\alpha+M'-r)} \Omega(\lambda; r, \alpha+M'-r)$$
$$= 1 + \lambda \sum_{r=2m-1}^{M'-2m} e^{-u((\alpha+1)+(M'-1)-r)} \Omega(\lambda; r, (\alpha+1)+(M'-1)-r)$$
$$+ \lambda e^{-u(\alpha+2m)} \Omega(\lambda; M'-2m, \alpha+2m)$$
$$= \Omega(\lambda, M'-1, \alpha+1) + \lambda e^{-u(\alpha+2m)} \Omega(\lambda; M'-2m, \alpha+2m) \qquad \text{(C.10)}$$

Proof of Lemma C.2. We prove the proposition (i) by complete induction with respect to s. For $s = 2m$ we have

$$\phi(\lambda; M, 2m) = \frac{\Omega(\lambda; M, 0)}{\Omega(\lambda; 2m-1, 0)} [1 - t_m(2m)] \qquad \text{(C.11)}$$

With $\Omega(\lambda; 2m-1, 0) = 1$, $t_m(2m) = \sum_{j=0}^{2m-1} \tilde{p}_{2m-j} = \tilde{p}_{2m}$ (note that $\tilde{p}_i = 0$ for $i < 2m$, and $\tilde{p}_{2m} = \lambda e^{-u(2m)} \Omega(\lambda; M-2m, 2m)/\Omega(\lambda; M, 0)$) it follows

$$\phi(\lambda; M, 2m) = \Omega(\lambda; M, 0) - \lambda e^{-u(2m)} \Omega(\lambda; M-2m, 2m) \qquad \text{(C.12)}$$

For $M' = M$ and $\alpha = 0$ we then obtain by using Lemma C.1 (ii)

$$\Omega(\lambda, M, 0) = \Omega(\lambda, M-1, 1) + \lambda e^{-u(2m)}\Omega(\lambda; M-2m, 2m) \tag{C.13}$$

and hence

$$\phi(\lambda; M, 2m) = \Omega(\lambda, M, 0) - \lambda e^{-u(2m)}\Omega(\lambda; M-2m, 2m) = \Omega(\lambda, M-1, 1) \tag{C.14}$$

Accordingly, proposition (i) is valid for $s = 2m$. Let us now assume that (i) holds true for $s-1 \geqslant 2m-1$.

Since $t_m(s) = \sum_{j=0}^{2m-1} \tilde{p}_{s-j}$ and $\tilde{p}_l = \lambda e^{-u(l)}\Omega(\lambda; l-1, 0)\, \Omega(\lambda; M-l, l)/\Omega(\lambda; M, 0)$ we can write

$$\begin{aligned}
\phi(\lambda; M, s) = {} & \frac{\Omega(\lambda; M, 0)}{\Omega(\lambda; s-1, 0)} \\
& \times \left[1 - \sum_{j=0}^{2m-1} e^{-u(s-j)}\, \lambda\, \frac{\Omega(\lambda; s-j-1, 0)\, \Omega(\lambda; M-s+j, s-j)}{\Omega(\lambda; M, 0)} \right] \\
= {} & \frac{1}{\Omega(\lambda; s-1, 0)} \left[\Omega(\lambda; M, 0) - \lambda \sum_{j=0}^{2m-1} e^{-u(s-j)} \right. \\
& \left. \times\, \Omega(\lambda; s-j-1, 0)\, \Omega(\lambda; M-s+j, s-j) \right] \\
= {} & \frac{1}{\Omega(\lambda; s-1, 0)} \left[\Omega(\lambda; M, 0) - \lambda \sum_{j=0}^{2m-1} e^{-u(s-1-j)}\Omega \right. \\
& \left. \times\, (\lambda; s-j-2, 0)\, \Omega(\lambda; M-s+1+j, s-1-j) \right] \\
& + \frac{\lambda}{\Omega(\lambda; s-1, 0)} [e^{-u(s-2m)}\Omega(\lambda; s-2m-1, 0) \\
& \times\, \Omega(\lambda; M-s+2m, s-2m) \\
& - e^{-u(s)}\Omega(\lambda; s-1, 0)\, \Omega(\lambda; M-s, s)] \\
= {} & \frac{1}{\Omega(\lambda; s-1, 0)} [\Omega(\lambda; s-2, 0)\, \phi(\lambda; M, s-1) \\
& + \lambda e^{-u(s-2m)}\Omega(\lambda; s-2m-1, 0)\, \Omega(\lambda; M-s+2m, s-2m)] \\
& - \lambda e^{-u(s)}\Omega(\lambda; M-s, s)
\end{aligned} \tag{C.15}$$

where the line 3 follows from line 2 after some straightforward manipulation of the sum over j, and line 4 from line 3 by definition of $\phi(\lambda; M, s-1)$.

Due to the induction hypothesis, $\phi(\lambda; M, s-1) = \Omega(\lambda; M-s+2m, s-2m)$, from which follows

$$\begin{aligned}\phi(\lambda; M, s) = {} & \frac{\Omega(\lambda; M-s+2m, s-2m)}{\Omega(\lambda; s-1, 0)} \\ & \times [\Omega(\lambda; s-2, 0) + \lambda e^{-u(s-2m)}\Omega(\lambda; s-2m-1, 0)] \\ & - \lambda e^{-u(s)}\Omega(\lambda; M-s, s)\end{aligned} \tag{C.16}$$

By using (i) of Lemma C.1 for $M' = s-1$ and $\alpha = 0$ we obtain

$$\Omega(\lambda; s-1, 0) = \Omega(\lambda; s-2, 0) + \lambda e^{-u(s-2m)}\Omega(\lambda; s-2m-1, 0) \tag{C.17}$$

and hence

$$\phi(\lambda; M, s) = \Omega(\lambda, M-s+2m, s-2m) - \lambda e^{-u(s)}\Omega(\lambda; M-s, s) \tag{C.18}$$

By using (ii) of Lemma C.1. for $M' = M-s+2m$ and $\alpha = s-2m$ we find

$$\begin{aligned}& \Omega(\lambda; M-s+2m, s-2m) \\ & \quad = \Omega(\lambda; M-s+2m-1, s-2m+1) + \lambda e^{-u(s)}\Omega(\lambda; M-s, s)\end{aligned} \tag{C.19}$$

and hence

$$\begin{aligned}\Omega(\lambda; M-s+2m, s-2m) - \lambda e^{-u(s)}\Omega(\lambda; M-s, s) \\ = \Omega(\lambda; M-s+2m-1, s-2m+1) \\ = \phi(\lambda; M, s)\end{aligned} \tag{C.20}$$

This completes the proof of part (i) of Lemma C.2.

To proof the second part (ii), we apply (ii) of Lemma C.1. For $M' = M-s+2m$ and $\alpha = s-2m$ we obtain

$$\begin{aligned}& \Omega(\lambda; M-s+2m, s-2m) \\ & \quad = \Omega(\lambda; M-s+2m+1, s-2m+1) + \lambda e^{-u(s)}\Omega(\lambda; M-s, s)\end{aligned} \tag{C.21}$$

Due to part (i) of the Lemma just proven, $\phi(\lambda; M, s) = \Omega(\lambda; M-s+2m-1, s-2m+1)$ and $\phi(\lambda; M, s-1) = \Omega(\lambda; M-s+2m, s-2m)$. Inserting this in (C.21) it follows proposition (ii).

Proof of Theorem C.1. According to Lemma C.2. and the definitions of $\tilde{p}_s$ and $t_m(s)$,

$$1 - t_m(s) + \tilde{p}_s = \frac{\Omega(\lambda; s-1, 0)}{\Omega(\lambda; M, 0)} [\phi(\lambda; M, s) + \lambda e^{-u(s)} \Omega(\lambda; M-s, s)]$$

$$= \frac{\Omega(\lambda; s-1, 0)}{\Omega(\lambda; M, 0)} \phi(\lambda; M, s-1) \tag{C.22}$$

Since $\Omega(\lambda; s-1, 0) = 0$ for $s < 2m$ and $\Omega(\lambda; M-s, s) = 0$ for $s > M+1-2m$, it follows $\tilde{p}_s = 0$ for $s \notin \{2m,..., M+1-2m\}$. For $s \in \{2m,..., M+1-2m\}$ on the other hand, we obtain from Lemma C.2 and Eqs. (C.2), (C.3), (C.22)

$$0 = -\log \lambda + u(l) + \log \left[\lambda e^{-u(l)} \frac{\Omega(\lambda; s-1, 0)\, \Omega(\lambda, M-l, l)}{\Omega(\lambda; M, 0)} \right]$$

$$+ \sum_{s=l+1}^{l+2m-1} \log \left[\frac{\Omega(\lambda; s-1, 0)}{\Omega(\lambda; M, 0)} \phi(\lambda; M, s-1) \right]$$

$$- \sum_{s=l}^{l+2m-1} \log \left[\frac{\Omega(\lambda; s-1, 0)}{\Omega(\lambda; M, 0)} \phi(\lambda; M, s) \right]$$

$$= \log \Omega(\lambda; M-l, l) - \log \phi(\lambda; M, l+2m-1)$$

$$= 0 \tag{C.23}$$

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