Stony Brook University

OFFICIAL COPY

The official electronic file of this thesis or dissertation is maintained by the University Libraries on behalf of The Graduate School at Stony Brook University.

© All Rights Reserved by Author.

Statistical mechanics of hard spheres and the two dimensional Ising lattice

A Dissertation Presented

by

Ivar Lyberg

to

The Graduate School

in Partial Fullfillment of the

Requirements

for the Degree of

Doctor of Philosophy

in

Mathematics

Stony Brook University

May 2007

Stony Brook University

The Graduate School

Ivar Lyberg

We, the dissertation committee for the above candidate for the

Doctor of Philosophy degree, hereby recommend

acceptance of this dissertation.

Prof. Barry M. McCoy, Institute for Theoretical Physics

Prof. Christopher Bishop, Department of Mathematics

Prof. Leon Takhtajan, Department of Mathematics

Prof. Vladimir Korepin, Institute for Theoretical Physics

This dissertation is accepted by the Graduate School

Lawrence Martin
Dean of the Graduate School

Abstract of the Dissertation

Statistical mechanics of hard spheres and the two dimensional Ising lattice

by

Ivar Lyberg

Doctor of Philosophy

in

Mathematics

Stony Brook University

2007

In this dissertation the fourth virial coefficient of a fluid of hard spheres in dimensions 5, 7, 9, and 11 is calculated. Furthermore, the complete star of n points in dimension 2 is reduced to an $n-2$-fold integral. Finally, the row and diagonal correlation functions of the two dimensional Ising lattice are computed as form factor expansions.

Contents

I. INTRODUCTION

This thesis treats the hard sphere model and the two dimensional Ising lattice. Thermodynamical properties will be calculated exactly. The pressure P of a fluid of hard disks will be calculated in terms of the density exactly as a power series.

The two dimensional Ising model is the most completely studied exactly solvable model. One of the unresolved problems is the calculation of the correlation function $\langle\sigma_{00}\sigma_{MN}\rangle$. Here $\langle\sigma_{00}\sigma_{0N}\rangle$ and $\langle\sigma_{00}\sigma_{NN}\rangle$ will be calculated exactly as series.

The two topics will be treated separately. Sections II A, II B and II C have been published in Journal of Statistical Physics [1], and chapter III has been published in Journal of Physics A [2].

A. Hard spheres

We consider the low density expansion of a fluid of N D-dimensional hard spheres. The position of the ith particle is $\mathbf{r}_i \in \mathbf{R}^D$, and the distance between two points is $r_{ij} := |\mathbf{r}_i - \mathbf{r}_j|$. The pair potential $\phi(r_{ij})$ is

$$\phi(r_{ij}) = \begin{cases} \infty & \text{if } r_{ij} \leq \sigma \\ 0 & \text{if } r_{ij} > \sigma, \end{cases} \tag{1}$$

where σ is some distance. The Hamiltonian is

$$H_N = \sum_{1\leq i<j\leq N} \phi(r_{ij}) + \sum_{i=1}^{N} \frac{p_i^2}{2m}. \tag{2}$$

Let $\{U_j\}_{j=1}^{\infty}$ be a sequence of bounded subsets of $\mathbf{R}^D$ such that $U_j \subset U_{j+1}$ and $\bigcup_{j=1}^{\infty} U_j = \mathbf{R}^D$, and let $\{N_j\}_{j=1}^{\infty} \subset \mathbf{N}$ be another sequence. $\{U_j\}_{j=1}^{\infty}$ and $\{N_j\}_{j=1}^{\infty}$ are chosen so that $N_j/|U_j| = \rho$, where the density ρ is independent of j and $|U_j|$ is the measure of U_j. The limit $j \to \infty$ is called the thermodynamic limit. In order for relevant quantities to exist in this limit it is necessary that $\lim_{j\to\infty} |\partial U_j|/|U_j| = 0$, where ∂U_j is the boundary of U_j.

In the thermodynamic limit, the pressure P of a fluid of hard spheres in D dimensions has a power series representation

$$\frac{P}{kT} = \rho + \sum_{n=2}^{\infty} B_n^{(D)} \rho^n. \tag{3}$$

Penrose and Lebowitz [3] have shown that the right hand side of (3) has a radius of convergence $R^{(D)}$ with a lower bound

$$R^{(D)} \geq \frac{1}{B_2^{(D)}} \max_{0 \leq w \leq 1} w(2e^{-w} - 1) = \frac{0.1446...}{B_2^{(D)}}. \tag{4}$$

There are several systematic ways to formalise the calculation of the virial coefficients $B_n^{(D)}$. One of these methods is the Mayer expansion [4], [5]. In this expansion a function called the Mayer f function is defined:

$$f(r_{ij}) := e^{-\phi(r_{ij})/kT} - 1. \tag{5}$$

Since ϕ is given by (1), it follows that

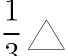
$$f_{ij} := f(r_{ij}) = \begin{cases} -1 & \text{if } r_{ij} \leq \sigma \\ 0 & \text{if } r_{ij} > \sigma. \end{cases} \tag{6}$$

The virial coefficients are given by [5]

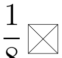
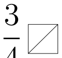
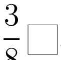
$$B_{n+1}^{(D)} = -\lim_{j \to \infty} \frac{n}{n+1} \frac{1}{n!|U_j|} \prod_{i=1}^{n} \int_{U_j} d^D \mathbf{r}_i V_{n+1}(\mathbf{r}_1, ..., \mathbf{r}_n) \tag{7}$$

where V_{n+1} is the collection of labelled biconnected Mayer diagrams with n points. Each bond of these diagrams represents a function $f(r_{ij})$ in the integrand of (7). Explicitly

$$B_2 = -\frac{1}{2} \int_{\mathbf{R}^D} f(r_{12}) d^D \mathbf{r}_2 = -\frac{1}{2}$$  , (8)

$$B_3 = -\frac{1}{3} \int_{\mathbf{R}^D} \int_{\mathbf{R}^D} f(r_{12}) f(r_{13}) f(r_{23}) d^D \mathbf{r}_2 d^D \mathbf{r}_3 = -\frac{1}{3}$$  , (9)

and

$$B_4 = -\frac{1}{8}$$  $$-\frac{3}{4}$$  $$-\frac{3}{8}$$  . (10)

From now on, we will usually disregard the superscript D and write B_n, and we will let $\sigma = 1$.

If the hard sphere potential (1) is considered, B_2 and B_3 can easily be explicitly evaluated. The second virial coefficient in three dimensions was first computed by

TABLE I: The second and third virial coefficients

D	B_2	B_3/B_2^2	decimal expansion
2	$\pi/2$	$4/3 - \sqrt{3}/\pi$	0.78200...
3	$2\pi/3$	$5/8$	0.625
4	$\pi^2/4$	$4/3 - (3/2)\sqrt{3}/\pi$	0.50634...
5	$4\pi^2/15$	$53/2^7$	0.41406...
6	$\pi^3/12$	$4/3 - (9/5)\sqrt{3}/\pi$	0.34094...
7	$8\pi^3/105$	$289/2^{10}$	0.28222...
8	$\pi^4/48$	$4/3 - (279/140)\sqrt{3}/\pi$	0.23461...

van der Waals [6] and the third was calculated independently by Boltzmann [7] and Jäger [8]. The second virial coefficient in dimension D is given by the function

$$B_2 = \frac{\pi^{D/2}}{2\Gamma(D/2+1)}, \tag{11}$$

and the third virial coefficient in dimension D is given by [43]

$$\frac{B_3}{B_2^2} = \frac{4\Gamma(1+D/2)}{\pi^{1/2}\Gamma((1+D)/2)} \int_0^{\pi/3} \sin^D \varphi \, d\varphi. \tag{12}$$

Table I shows the values of the second and third virial coefficients in dimensions two to eight.

The history of the computation of $B_4^{(3)}$ dates back to the end of the nineteenth century [9]. Van der Waals [6] formulated a sum of integrals which he thought would give B_4. However, there was one integral which he could not evaluate (This was the one which is today called the complete star of four points, written $\boxtimes$ in (10)). Van Laar evaluated this integral and published his result in 1899 [10]. Boltzmann contested van der Waals' formulation of the problem; today we would say that his version of (10) had the wrong coefficients. Using the correct virial series expansion (10), Boltzmann published the correct result in the same year [11]. His result was

$$\frac{B_4}{B_2^3} = \frac{2707}{4480} + \frac{219}{2240}\frac{\sqrt{2}}{\pi} - \frac{4131}{4480}\frac{\arccos(1/3)}{\pi} = 0.28694950598\ldots\,. \tag{13}$$

This result was confirmed in 1952 by Nijboer and van Hove [12] using what is called the two center formalism [13]. The two center formalism is a formalism different from

(7), and is useful mainly for the hard sphere potential. It will be presented in detail in chapter II.

The calculation of $B_4^{(2)}$ was done by Rowlinson in 1964 [14] (using the Mayer formalism (7)) and independently by Hemmer in 1965 [15]. Their result was

$$\frac{B_4}{B_2^3} = 2 - \frac{9}{2}\frac{\sqrt{3}}{\pi} + 10\frac{1}{\pi^2} = 0.53223180... \, . \tag{14}$$

Clisby and McCoy [16] calculated $B_4^{(D)}$ for $D = 4, \ 6, \ 8, \ 10$ and 12, using the Mayer formalism. Their results are shown in table II.

TABLE II: Exact values of the fourth virial coefficient in low even dimensions

D	B_4/B_2^3	decimal expansion
4	$2 - \frac{27}{4}\frac{\sqrt{3}}{\pi} + \frac{832}{45}\frac{1}{\pi^2}$	0.15184606235...
6	$2 - \frac{81}{10}\frac{\sqrt{3}}{\pi} + \frac{38848}{1575}\frac{1}{\pi^2}$	0.03336314...
8	$2 - \frac{2511}{280}\frac{\sqrt{3}}{\pi} + \frac{17605024}{606375}\frac{1}{\pi^2}$	−0.00255768...
10	$2 - \frac{2673}{280}\frac{\sqrt{3}}{\pi} + \frac{49048616}{1528065}\frac{1}{\pi^2}$	−0.01096248...
12	$2 - \frac{2187}{220}\frac{\sqrt{3}}{\pi} + \frac{11565604768}{337702365}\frac{1}{\pi^2}$	−0.010670281...

The virial coefficient $B_4^{(D)}$ in odd dimensions has previously been computed by Monte Carlo methods by Ree and Hoover [17] and Clisby and McCoy [18]. These numerical results gave the first demonstration that the hard sphere virial coefficients can be negative. The question of negativity of hard sphere virial coefficients is of great theoretical importance, and in dimensions $D \leq 4$ Monte Carlo investigations have thus far seen only positive $B_n^{(D)}$ for $n \leq 10$.

The study of virial coefficients in higher dimensions is important. There is a change of sign of $B_4^{(D)}$ at $D \approx 7.7$ [18], and this has important implications. If $B_n^{(D)}$ oscillates in sign with some period for large n, then the first singularity will occur off the real axis.

One reason to seek exact values of the virial coefficients is that approximate values may require more computer power than is available. For instance, no one has so far been able to calculate sufficiently many virial coefficients to produce the expected phase transition at some critical density. It may be that the radius of convergence of the power series (3) is less than the density of the phase transition, in which case nothing can be learned about the phase transition by calculating a finite number of virial coefficients. Even if the radius were greater than the critical density, it seems unlikely that a sufficient number of virial coefficients will be calculated in the near future. See, for instance, Clisby and McCoy [18].

1. Summary of results

In this thesis, in chapter II, we calculate the exact values of $B_4^{(D)}$ for $D = 5,\ 7,\ 9$ and 11. The results are shown in table III. It is seen that the results agree with previous numerical calculations [19] [20] [18].

TABLE III: Exact and numerical values of the fourth virial coefficient in low odd dimensions

D	B_4/B_2^3	decimal expansion
5	$\frac{25315393}{32800768} + \frac{3888425}{16400384}\frac{\sqrt{2}}{\pi} - \frac{67183425}{32800768}\frac{\arccos(1/3)}{\pi}$	0.07597248028...
		0.075972512(4) [19]
		0.07592(6) [20]
		0.075978(4) [18]
7	$\frac{299189248759}{290596061184} + \frac{159966456685}{435894091776}\frac{\sqrt{2}}{\pi} - \frac{292926667005}{96865353728}\frac{\arccos(1/3)}{\pi}$	0.00986494662...
		0.009873(3) [18]
9	$\frac{2886207717678787}{2281372811001856} + \frac{2698457589952103}{5703432027504640}\frac{\sqrt{2}}{\pi} - \frac{8656066770083523}{2281372811001856}\frac{\arccos(1/3)}{\pi}$	$-0.00858079817...$
		$-0.008575(3)$ [18]
11	$\frac{17357449486516274011}{11932824186709344256} + \frac{16554115383300832799}{29832060466773360640}\frac{\sqrt{2}}{\pi}$	
	$-\frac{52251492946866520923}{11932824186709344256}\frac{\arccos(1/3)}{\pi}$	$-0.01133719858...$
		$-0.011333(3)$ [18]

The calculation of coefficients of order higher than four can be reduced to a problem in computational algebraic geometry. We will consider only the complete star. The complete star of n points is the graph of n points where each point is is directly connected with every other point. In section II E we will define a function $\chi_n(r)$ such that $\chi_n(1)$ is equivalent to the complete star of n points. It will be shown that

$$\chi_{n+2}(r) = \frac{(-1)^{n(n-1)/2}}{2^{n(n-3)}} \prod_{i=1}^{n} \int_0^{1-r/2} dz_i \prod_{j=1}^{n} \int_0^{\sqrt{1-(r/2+z_j)^2}} ds_j \sum_{\sigma\in\{-1,1\}^{(n-1)n/2}} \prod_{1\le k<l\le n} \left(1 + \mathbf{1}_{[s_k+s_l<\sqrt{1-(\sigma_k z_k - \sigma_l z_l)^2}]}\right) \tag{15}$$

where

$$\mathbf{1}_A(x) := \begin{cases} 1 \text{ if } x \in A \\ 0 \text{ if } x \notin A. \end{cases} \tag{16}$$

The following conjecture is proposed.

Conjecture 1 In even dimensions, the normalized nth virial coefficient B_n/B_2^{n-1} can be written as

$$\frac{B_n}{B_2^{n-1}} = \sum_{j=0}^{n-2} a_j(\sqrt{3}/\pi)^j, \tag{17}$$

where the coefficients a_j are rational numbers.

This is known to be true for the second, third and fourth virial coefficients. It is shown in section II that the nth virial coefficient in two dimensions may be written as an $n-2$ dimensional integral over a region bounded by certain algebraic varieties. These integrals have not yet been evaluated.

B. The two dimensional Ising lattice

We consider a rectangular spin lattice with $\mathcal{M}\times\mathcal{N}$ lattice points, where each lattice point (i,j) has two possible spin states ($\sigma_{ij} = \pm 1$). The interaction energy between two neighboring spins sites (i,j) and $(i+1,j)$ is $-E_1\sigma_{ij}\sigma_{i+1,j}$, and the interaction energy between two neighboring spins sites (i,j) and $(i,j+1)$ is $-E_2\sigma_{ij}\sigma_{i,j+1}$ where $E_j = K_j kT$ (k is Boltzmann's constant, T is the temperature and K_1 and K_2 are positive constants). We impose toroidal boundary conditions, so that $(i,\mathcal{N}) \equiv (i,0)$ and $(\mathcal{M},j) \equiv (0,j)$. Thus the total interaction energy is

$$E_{\mathcal{M},\,\mathcal{N}}(\sigma) = -\sum_{i=0}^{\mathcal{M}-1}\sum_{j=0}^{\mathcal{N}-1}(E_1\sigma_{ij}\sigma_{i+1,j} + E_2\sigma_{ij}\sigma_{i,j+1}). \tag{18}$$

The partition function is

$$Z_{\mathcal{M},\,\mathcal{N}} = \sum_{\sigma} \exp -E_{\mathcal{M},\,\mathcal{N}}(\sigma)/kT. \tag{19}$$

The Gibbs free energy per site is defined to be

$$f_{\mathcal{M},\,\mathcal{N}} := -\frac{kT}{\mathcal{M}\mathcal{N}} \log Z_{\mathcal{M},\,\mathcal{N}}. \tag{20}$$

We define

$$f := \lim_{\mathcal{M},\,\mathcal{N}\to\infty} f_{\mathcal{M},\,\mathcal{N}}. \tag{21}$$

The correlation function $\langle\sigma_{0,0}\sigma_{M,N}\rangle_{\mathcal{M},\,\mathcal{N}}$ is defined to be

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle_{\mathcal{M},\mathcal{N}} := \frac{1}{Z_{\mathcal{M},\mathcal{N}}} \sum_{\sigma} \sigma_{0,0}\sigma_{M,N} \exp -E_{\mathcal{M},\,\mathcal{N}}(\sigma)/kT, \tag{22}$$

and the correlation function $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ is defined to be

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle := \lim_{\mathcal{M},\,\mathcal{N}\to\infty} \langle\sigma_{0,0}\sigma_{M,N}\rangle_{\mathcal{M},\,\mathcal{N}}. \tag{23}$$

We will consider only the special cases $M = 0$ and $M = N$.

The correlation functions $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ of the two dimensional Ising model with horizontal (vertical) interaction energies E_1 (E_2) can be written in many different ways which appear to be different but which in fact are equal. They were first expressed as determinants by Kaufman and Onsager [21]. Later Montroll, Potts and Ward [22] demonstrated that if an arbitrary path is drawn on the lattice connecting the point $(0,0)$ with the point (M,N) then the correlation can be expressed as a determinant whose size in general is twice the length of the path. The correlations $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ and $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ can both be expressed as $N\times N$ Toeplitz determinants [21]–[23], and expressions of $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ as determinants of size M and $M+1$ for $M \geq N$ were given by Yamada [24], [25]. Furthermore the correlations $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ for all finite $M,\ N$ were expressed as determinants of Fredholm operators by Cheng and Wu [26].

The representations of the correlations as finite size determinants gives an efficient evaluation when the separation is small but to investigate the large separation behavior alternative representations are needed. The first such result is the limiting behavior for $T < T_c$

$$\begin{aligned} S_\infty = &\lim_{N\to\infty} \langle\sigma_{00}\sigma_{0N}\rangle = \lim_{N\to\infty} \langle\sigma_{00}\sigma_{NN}\rangle \\ = &\left\{1 - (\sinh 2E_1/kT \sinh 2E_2/kT)^{-2}\right\}^{1/4}, \end{aligned} \tag{24}$$

which is most easily computed [22] by the use of Szegö's theorem [27],[28].

The first large separation expansion for both $T < T_c$ and $T > T_c$ beyond the limiting value (24) was given in 1966 by Wu [29] for $\langle \sigma_{00}\sigma_{0N} \rangle$ by applying a Wiener-Hopf procedure to the $N \times N$ Toeplitz determinant representation. Shortly thereafter Cheng and Wu [26] obtained the leading term of the large separation behavior of $\langle \sigma_{00}\sigma_{MN} \rangle$ by applying a Wiener-Hopf procedure to the Fredholm determinant representation. This derivation is formally valid only for $M \neq 0$, and even though it is expected that the result of [26] with M formally set equal to zero should agree with the result of [29], there is no analytic derivation in the literature that for $T < T_c$ the two results are in fact equal (even though the equality has been verified to large orders in the low temperature expansion.)

The expansions of [29] and [26] may be considered as the first terms in a systematic expansion of the correlations. The expansion technique of [26] which starts from the Fredholm determinant representation was carried out to all orders by Wu, McCoy, Tracy and Barouch [30] in 1976. It was found that the correlations can be written in the following exponential form

$$\langle \sigma_{00}\sigma_{MN} \rangle_{T<T_c} = S_\infty \exp \sum_{n=1}^{\infty} F_{MN}^{(2n)} \quad \text{for } T < T_c \tag{25}$$

and as

$$\langle \sigma_{00}\sigma_{MN} \rangle_{T>T_c} = \widehat{S}_\infty \sum_{m=0}^{\infty} G_{MN}^{(2m+1)} \exp \sum_{n=1}^{\infty} \widehat{F}_{MN}^{(2n)} \quad \text{for } T > T_c \tag{26}$$

where

$$\widehat{S}_\infty = \left\{1 - (\sinh 2E_1/kT \sinh 2E_2/kT)^2\right\}^{1/4}. \tag{27}$$

In [30] the expressions for $F_{MN}^{(j)}$, $\widehat{F}_{MN}^{(j)}$ and $G_{MN}^{(j)}$ are given as $2j$ fold multiple dimensional integrals.

The exponentials in (25) and (26) may be expanded to give what is called a form factor expansion

$$\langle \sigma_{00}\sigma_{MN} \rangle_{T<T_c} = S_\infty \sum_{n=0}^{\infty} f_{MN}^{(2n)} \quad \text{for } \; T < T_c \tag{28}$$

and

$$\langle \sigma_{00}\sigma_{MN} \rangle_{T>T_c} = \widehat{S}_\infty \sum_{n=0}^{\infty} f_{MN}^{(2n+1)} \quad \text{for } \; T > T_c. \tag{29}$$

The first few terms in this expansion were given in [30]. In the scaling limit $N \to \infty$, $T \to T_c$ with $N|T - T_c|$ fixed the full expansion was given by Nappi [31]. For fixed N and $T < T_c$ the full expansion (28) was given by Palmer and Tracy [32]. Both of the cases $T < T_c$ and $T > T_c$ were treated by Nickel [33]-[34]. An independent expansion was given by Yamada [35], and this is shown in [34] to agree with the results from the expansion of the exponential forms of [30].

The results for the exponential representation of the correlations [30] were obtained by extending to all orders the interative expansion of the Fredholm determinant representation [26]. However, as noted above, the result of [26] for $F^{(2)}_{M,N}$ when specialized to $M = 0$ "looks different" from the corresponding result for $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ obtained in [29]. Moreover the leading order large N behavior of $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ is obtained [36] from the results for of [29] for $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ and this result looks very different from the result of [30]. Therefore it must be the case that if the Wiener-Hopf procedure of Wu [29], which starts from the $N \times N$ Toeplitz determinant representation of $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ and $\langle\sigma_{0,0}\sigma_{N,N}\rangle$, is iterated to all orders we will obtain a representation of $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ and $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ which is different from that of ref. [30].

In subsection I B 1 we summarize the results of our calculations. In section III B we calculate the exponential representation of the correlation functions $\langle\sigma_{00}\sigma_{0N}\rangle$ and $\langle\sigma_{00}\sigma_{NN}\rangle$ for $T < T_c$. In section III C we calculate the exponential representations for $T > T_c$. In section III D we calculate the form factor expansions of $\langle\sigma_{00}\sigma_{0N}\rangle$ and $\langle\sigma_{00}\sigma_{NN}\rangle$ for $T < T_c$ and section III E we calculate the form factor expansions for $T > T_c$, We conclude in sec. III F with a brief discussion of our results.

In chapter III we calculate the correlation functions $\langle\sigma_{00}\sigma_{0N}\rangle$ and $\langle\sigma_{00}\sigma_{NN}\rangle$ as series

$$D_N = \begin{cases} D_N^{(-)} = \sum_{n=0}^{\infty} f_N^{(2n)} & \text{if } T < T_c \\ D_N^{(+)} = \sum_{n=0}^{\infty} f_N^{(2n+1)} & \text{if } T > T_c. \end{cases} \tag{30}$$

The functions $f_N^{(2n)}$ are called form factors, and are $2n$ dimensional integrals.

We let D_N stand for $S_N = \langle\sigma_{00}\sigma_{0N}\rangle$ or $C_N = \langle\sigma_{00}\sigma_{NN}\rangle$. Then

$$D_N = \begin{cases} D_N^{(-)} & \text{for } T < T_c \\ D_N^{(+)} & \text{for } T > T_c \end{cases} \tag{31}$$

The representation of these correlations as an $N \times N$ Toeplitz determinant is [36]

$$D_N = \det \mathbf{A}_N \tag{32}$$

where

$$\mathbf{A}_N = \begin{pmatrix} a_0 & a_{-1} & \dots & a_{1-N} \\ a_1 & a_0 & \dots & a_{2-N} \\ \vdots & \vdots & \ddots & \vdots \\ a_{N-1} & a_{N-2} & \dots & a_0 \end{pmatrix} \tag{33}$$

and

$$a_n = \frac{1}{2\pi i}\oint_{|z|=1} \varphi(z) z^{-n-1}\, dz, \tag{34}$$

where the path of integration is counterclockwise. The function $\varphi(z)$ is

$$\varphi(z) = \left(\frac{(1-\alpha_1 z)(1-\alpha_2 z^{-1})}{(1-\alpha_1 z^{-1})(1-\alpha_2 z)}\right)^{1/2}. \tag{35}$$

For the diagonal correlation function C_N

$$\alpha_1 = 0 \quad \text{and} \quad \alpha_2 = (\sinh 2K_1 \sinh 2K_2)^{-1} \tag{36}$$

where $K_j = E_j/kT$. For the row correlation function S_N

$$\alpha_1 = e^{-2K_2}\tanh K_1 \quad \text{and} \quad \alpha_2 = e^{-2K_2}\coth K_1. \tag{37}$$

We will prove in Sec. III B that the correlation function $D_N^{(-)}$ has an exponential expansion

$$D_N^{(-)} = S_\infty \exp \sum_{n=1}^{\infty} F_N^{(2n)} \tag{38}$$

where

$$S_\infty = \left[\frac{(1-\alpha_1^2)(1-\alpha_2^2)}{(1-\alpha_1\alpha_2)^2}\right]^{1/4} \tag{39}$$

which for both the diagonal (36) and row (37) correlation function specializes to (24). The function $F_N^{(2n)}$ is given by

$$F_N^{(2n)} = \frac{(-1)^{n+1}}{n(2\pi)^{2n}} \lim_{\epsilon\to 0} \prod_{i=1}^{2n} \oint_{|z_i|=1-\epsilon} dz_i \prod_{j=1}^{2n} \frac{z_j^N}{1-z_j z_{j+1}} \prod_{k=1}^{n} P(z_{2k})P(z_{2k}^{-1})Q(z_{2k-1})Q(z_{2k-1}^{-1}) \tag{40}$$

where $z_{2n+1} = z_1$ and the functions $P(z)$ and $Q(z)$ are

$$P(z) = ((1-\alpha_2 z)/(1-\alpha_1 z))^{1/2} \tag{41}$$

and

$$Q(z) = ((1-\alpha_1 z)/(1-\alpha_2 z))^{1/2} = 1/P(z). \tag{42}$$

This agrees with the result given in ref. [37] for the diagonal correlation function $C_N^{(-)}$.

In Sec. III D we prove that $D_N^{(-)}$ has the form factor expansion

$$D_N^{(-)} = S_\infty \sum_{n=0}^{\infty} f_N^{(2n)} \tag{43}$$

where $f_N^{(0)} = 1$ and

$$f_N^{(2n)} = \frac{1}{(n!)^2(2\pi)^{2n}} \lim_{\epsilon\to 0} \prod_{i=1}^{2n} \oint_{|z_i|=1-\epsilon} dz_i\ z_i^N \prod_{k=1}^{n} P(z_{2k})P(z_{2k}^{-1})Q(z_{2k-1})Q(z_{2k-1}^{-1}) \prod_{l=1}^{n}\prod_{m=1}^{n}(1-z_{2l-1}z_{2m})^{-2} \prod_{1\le p<q\le n} (z_{2p-1}-z_{2q-1})^2(z_{2p}-z_{2q})^2. \tag{44}$$

This agrees with the result given in ref. [37] for the diagonal correlation function $C_N^{(-)}$.

For $T > T_c$, we consider a new function $\widehat{\varphi}(z)$ such that

$$\widehat{\varphi}(z) = \varphi(z)z = \left(\frac{(1-\alpha_1 z)(1-\alpha_2^{-1}z)}{(1-\alpha_1 z^{-1})(1-\alpha_2^{-1}z^{-1})}\right)^{1/2} \tag{45}$$

which we write in factored form as

$$\widehat{\varphi}(z) = \widehat{P}(z)^{-1}\widehat{Q}(z^{-1})^{-1} \tag{46}$$

with

$$\widehat{P}(z) = ((1-\alpha_1 z)(1-\alpha_2^{-1}z))^{-1/2} \tag{47}$$

and

$$\widehat{Q}(z) = ((1-\alpha_1 z)(1-\alpha_2^{-1}z))^{1/2} = 1/\widehat{P}(z). \tag{48}$$

$\widehat{P}(z)$ and $\widehat{Q}(z)$ are analytic and non-zero for $|z| < 1$.

We prove in Sec. III C that the correlation function $D_N^{(+)}$ has an exponential expansion

$$D_N^{(+)} = -\widehat{S}_\infty \sum_{m=0}^{\infty} G_N^{(2m+1)} \exp \sum_{n=1}^{\infty} \widehat{F}_{N+1}^{(2n)} \tag{49}$$

where

$$\widehat{S}_\infty = \left[(1-\alpha_1^2)(1-\alpha_2^{-2})(1-\alpha_1\alpha_2^{-1})^2\right]^{1/4} \tag{50}$$

which for both the diagonal (36) and row (37) correlations specializes to (27) and where $\widehat{F}_N^{(2n)}$ is defined as in (40), but with P and Q replaced by $\widehat{P}$ and $\widehat{Q}$. Thus we find from (40) that $\widehat{F}_N^{(2n)}$ is

$$\begin{aligned}\widehat{F}_N^{(2n)} = \; & \frac{(-1)^{n+1}}{n(2\pi)^{2n}} \lim_{\epsilon\to 0} \prod_{i=1}^{2n} \oint_{|z_i|=1-\epsilon} dz_i \prod_{j=1}^{2n} \frac{z_j^N}{1-z_j z_{j+1}} \\ & \prod_{k=1}^{n} \widehat{P}(z_{2k})\widehat{P}(z_{2k}^{-1})\widehat{Q}(z_{2k-1})\widehat{Q}(z_{2k-1}^{-1}).\end{aligned} \tag{51}$$

The function $G_N^{(2n+1)}$ is given by

$$\begin{aligned}G_N^{(2n+1)} = \frac{1}{(2\pi i)^{2n+1}} \; & \lim_{\epsilon\to 0} \prod_{i=1}^{2n+1} \oint_{|z_i|=1-\epsilon} dz_i \; z_i^{N+1} \frac{1}{z_1 z_{2n+1}} \prod_{k=1}^{2n} \frac{1}{1-z_k z_{k+1}} \\ & \prod_{l=1}^{n+1} \widehat{P}(z_{2l-1})\widehat{P}(z_{2l-1}^{-1}) \prod_{m=1}^{n} \widehat{Q}(z_{2m})\widehat{Q}(z_{2m}^{-1}).\end{aligned} \tag{52}$$

Equations (51) and (52) agree with the results given in ref. [37]. Note that for the diagonal correlation function $C_N^{(+)} = \langle\sigma_{00}\sigma_{NN}\rangle$ (36) implies that

$$\widehat{F}_N^{(2n)} = F_N^{(2n)}. \tag{53}$$

In Sec. III E we prove that $D_N^{(+)}$ has the form factor expansion

$$D_N^{(+)} = -\widehat{S}_\infty \sum_{n=0}^{\infty} f_N^{(2n+1)} \tag{54}$$

where

$$\begin{aligned} f_N^{(2n+1)} = \quad & -\frac{i}{n!(n+1)!(2\pi)^{2n+1}} \lim_{\epsilon\to 0} \prod_{i=1}^{2n+1} \oint_{|z_i|=1-\epsilon} dz_i \; z_i^N \prod_{l=1}^{n+1} \widehat{P}(z_{2l-1})\widehat{P}(z_{2l-1}^{-1})z_{2l-1}^{-1} \\ & \prod_{m=1}^{n} \widehat{Q}(z_{2m})\widehat{Q}(z_{2m}^{-1})z_{2m} \prod_{p=1}^{n+1}\prod_{q=1}^{n} \frac{1}{(1-z_{2p-1}z_{2q})^2} \\ & \prod_{1\le j<k\le n+1} (z_{2j-1}-z_{2k-1})^2 \prod_{1\le r<s\le n} (z_{2r}-z_{2s})^2. \end{aligned} \tag{55}$$

Equation (55) agrees with result given in ref. [37] for the diagonal correlation function $C_N^{(+)}$.

The proofs of these results are not restricted to the Ising case where the generating function is given by (35) but with a suitable replacement for the factors S_∞ and $\widehat{S}_\infty$ are valid in more general cases, for example the XY model in a magnetic field [38]-[40]. The results (38)-(44) for $T < T_c$ are valid for any generating function $\varphi(z)$ where $\log\varphi(z)$ is analytic and periodic on $|z| = 1$ and $P(z) = 1/Q(z)$ The results (49)-(55) for $T > T_c$ are similarly valid for any generating function for which $\log z\varphi(z)$ is analytic and periodic on the unit circle $|z| = 1$ and $\widehat{P}(z) = 1/\widehat{Q}(z)$.

II. HARD SPHERES

A. Introduction

In this chapter we will prove the results (15) and table III. In section II B we review the relation between the two center formalism and the Mayer formalism. In section II C we prove the result presented in table III. In sections II D and II E we use the two center formalism to evaluate the complete star of $B_{n+2}^{(2)}$ in terms of $n$dimensional integrals. We conclude in section II F with a discussion.

The partition function may be written as

$$Z_{N_j} = \frac{1}{N_j! h^{DN_j}} \prod_{k=1}^{N_j} \int_{\mathbf{R}^D} d^D\mathbf{p}_k \prod_{l=1}^{N_j} \int_{U_j} d^D\mathbf{r}_l \ \exp -H_{N_j}/kT \tag{56}$$

where h is Planck's constant. After Gaussian integration (56) becomes

$$Z_{N_j} = \frac{1}{N_j! \lambda^{DN_j}} \prod_{l=1}^{N_j} \int_{U_j} d^D\mathbf{r}_l \ \exp -\frac{1}{kT} \sum_{1\leq i<k\leq N_j} \phi(r_{ik}) \tag{57}$$

where $\lambda := h/(2\pi mkT)^{1/2}$. With the definition (5), (57) becomes

$$Z_{N_j} = \frac{1}{N_j! \lambda^{DN_j}} \prod_{l=1}^{N_j} \int_{U_j} d^D\mathbf{r}_l \prod_{1\leq i<k\leq N_j} (1+f_{ik}). \tag{58}$$

A lengthy calculation [5] shows that the virial coefficients $B_n^{(D)}$ are given by (7). The integral in (12) for the virial coefficient $B_3^{(D)}$ may be evaluated easily. Let m be any positive integer, and let u be any positive number. According to reference [41], p. 159

$$\int_0^u \sin^{2m} x \ dx = \frac{(2m-1)!!}{2^m m!} u - \frac{\cos u}{2m} \times \Big\{ \sin^{2m-1} u + + \sum_{k=1}^{m-1} \frac{(2m-1)(2m-3)...(2m-2k+1)}{2^k (m-1)(m-2)...(m-k)} \sin^{2m-2k-1} u \Big\} \tag{59}$$

and

$$\int_0^u \sin^{2m+1} x \ dx = \frac{2^m m!}{(2m+1)(2m-1)!!} - \frac{\cos u}{2m+1} \Big\{ \sin^{2m} u + + \sum_{k=0}^{m-1} \frac{2^{k+1} m(m-1)...(m-k)}{(2m-1)(2m-3)...(2m-2k-1)} \sin^{2m-2k-2} u \Big\}. \tag{60}$$

The calculation of the fourth virial coefficient is more involved. The method used by Rowlinson [14] and Clisby and McCoy [16] was to calculate the volume of the intersection of three balls

$$v_D(r_{12}, r_{13}, r_{23}) = -\int_{\mathbf{R}^D} f(r_{14}) f(r_{24}) f(r_{34}) d^D\mathbf{r}_4 \tag{61}$$

as an intermediate step. It follows from (61) that

$$\boxtimes = -\int_{\mathbf{R}^D}\int_{\mathbf{R}^D}\int_{\mathbf{R}^D} f(r_{13}) f(r_{23}) f(r_{24}) v_D(r_{12}, r_{13}, r_{23}) d^D\mathbf{r}_1 d^D\mathbf{r}_2 d^D\mathbf{r}_3 \tag{62}$$

Rowlinson had previously calculated $v_3(r_{12}, r_{13}, r_{23})$ [42], but no one has so far calculated the three dimensional complete star using (62). The reason is that there are elliptic integrals in the odd dimensional case that cancel in the even dimensional case.

B. The two center formalism

The two center formalism was invented by de Boer in 1949 [13]. This formalism is equivalent [5] to the Mayer formalism, and in the case of hard spheres it especially useful since it allows the reduction of the dimension of the integral by D. The invention of this formalism is what inspired Nijboer and van Hove to confirm Boltzmann's result for $B_4^{(D)}$ in 1952 [12].

According to the Mayer formalism, $B_4^{(D)}$ is given by (10). If the pair potential is given by (1), then (and only then) the Mayer diagrams of B_4 can be written according to the two center formalism as

$$\begin{aligned} \boxtimes &= -4B_2 \boxtimes_{\circ\circ}(1) \\ \boxslash &= -\frac{4}{3}B_2\left(\frac{1}{2}\bowtie_{\circ\circ}(1) + 2\,\boxslash_{\circ\circ}(1)\right) \\ \square &= -\frac{8}{3}B_2 \sqcap_{\circ\circ}(1), \end{aligned} \tag{63}$$

and thus

$$B_4 = B_2\left(\frac{1}{2}\boxtimes_{\circ\circ}(1) + \frac{1}{2}\bowtie_{\circ\circ}(1) + 2\,\boxslash_{\circ\circ}(1) + \sqcap_{\circ\circ}(1)\right). \tag{64}$$

Here the circles indicate points that are not integrated over, and the number 1 indicates that the distance between these two points is 1. We shall use the same notation as Nijboer and van Hove [12]. Thus we define

$\chi(r_{12}) :=$ ,

$(g_1(r_{12}))^2 :=$ ,

$\psi(r_{12}) :=$ ,

$\varphi(r_{12}) :=$ . (65)

The functions $g_1(r_{12})$, $\varphi(r_{12})$ and $\psi(r_{12})$ are easily calculated for any D. The calculation of these diagrams in three dimensions is described in the paper by Nijboer and van Hove [12]. It is easy to do the same calculation in higher odd dimensions, but we shall omit this since the lower order Mayer diagrams in B_4 are already known in terms of hypergeometric functions. Luban and Baram [43] showed that

$$\frac{\square}{B_2^3} = \frac{2^{D+4}}{\pi} \frac{\Gamma(D+1)[\Gamma(D/2+1)]^3}{\Gamma(3D/2+1)[\Gamma((D+3)/2)]^2} {}_3F_2\left(\frac{1}{2}, 1, \frac{-D+1}{2}; \frac{D+3}{2}, \frac{D+3}{2}; 1\right) \quad (66)$$

and

$$\frac{\boxslash}{B_2^3} = -2^{D+1} D^3 [\Gamma(D/2)]^2 \int_0^1 dy\; y[g_{D/2}(y)]^2, \quad (67)$$

where

$$g_\nu(y) = \int_0^\infty dx\; x^{-\nu}[J_\nu(x)]^2 J_{\nu-1}(xy). \quad (68)$$

If D is odd, then according to reference [41], p. 1071

$$\begin{aligned} {}_3F_2\left(\frac{1}{2}, 1, \frac{-D+1}{2}; \frac{D+3}{2}, \frac{D+3}{2}; 1\right) &= \\ &= \sum_{k=0}^{n} (-1)^k \frac{(2k-1)!!}{2^k} \quad \frac{n(n-1)...(n-k+1)}{[(n+k+1)(n+k)...(n+2)]^2} \end{aligned} \quad (69)$$

where $D = 2n+1$ and $(-1)!! = (-1)^0 = 1$. Joslin [44] found that

$$g_\nu(y) = \begin{cases} \frac{2^{-\nu} y^{\nu-1}}{\Gamma(\nu+1/2)\Gamma(1/2)} \int_{2\arcsin(y/2)}^{\pi} d\varphi \;\cos^{2\nu}(\varphi/2) & \text{if } y < 2 \\ 0 & \text{if } y \geq 2. \end{cases} \quad (70)$$

Thus, if $y < 2$, n is a positive integer and $D = 2n+1$, then

$$\begin{aligned} g_{D/2}(y) = \quad & \frac{2^{-D/2} y^{D/2-1}}{\Gamma(n+1)\Gamma(1/2)} 2\Bigg(\frac{1}{2n+1} \frac{2^n n!}{(2n-1)!!} - \frac{y/2}{2n+1}\Bigg\{(1-(y/2)^2)^n + \\ & + \sum_{k=0}^{n-1} \frac{2^{k+1} n(n-1)...(n-k)}{(2n-1)(2n-3)...(2n-2k-1)} (1-(y/2)^2)^{n-k-1}\Bigg\}\Bigg). \end{aligned} \quad (71)$$

Thus using (69) and (70), the expressions in (66) and (67) can be explicitly computed in odd dimensions. Clearly both of these are rational numbers in odd dimensions.

C. Integration of the complete star

We aim to obtain a general expression for $\chi(1)$. The only dimensions lower than 12 for which the exact result has not been published before are $D = 5,\ 7,\ 9,\ 11$. We shall calculate χ in dimensions $D = 2n+1$. When n is an integer, D is an odd integer. However, n need not be an integer. If n is a half integer, then the calculation below is still valid and gives B_4 in even dimensions. If n is some other positive real number, then the calculation below may be used to obtain B_4 in continous dimensions. We will use the convention

$$r_{12} \geq 1. \tag{72}$$

According to (65)

$$\chi(r_{12}) = \int_{\mathbf{R}^D} \int_{\mathbf{R}^D} f(r_{13}) f(r_{14}) f(r_{23}) f(r_{24}) f(r_{34}) d^D\mathbf{r}_3 d^D\mathbf{r}_4 \tag{73}$$

We define

$$F(h) = \int_{\mathbf{R}^D} f(r_{ij}) e^{2\pi i \mathbf{h}\cdot(\mathbf{r}_i - \mathbf{r}_j)} d^D\mathbf{r}_i \tag{74}$$

where $h = |\mathbf{h}|$. It can be shown that [43]

$$F(h) = -\frac{1}{h^{D/2}} J_{D/2}(2\pi h) \tag{75}$$

where J_ν is a Bessel function of order ν. We define

$$G(\mathbf{h}, r_{12}) = \int_{\mathbf{R}^D} f(r_{13}) f(r_{23}) e^{2\pi i \mathbf{h}\cdot[\mathbf{r}_3 - \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)]} d^D\mathbf{r}_3. \tag{76}$$

Clearly

$$\chi(r_{12}) = \int_{\mathbf{R}^D} F(h) [G(\mathbf{h}, r_{12})]^2 d^D\mathbf{h} \tag{77}$$

In D dimensions, we write $\mathbf{r} = (x_1, x_2, ..., x_{D-1}, z) = (\mathbf{x}, z)$ and $\mathbf{h} = (\mathbf{h}_x, h_z)$. $\mathbf{r}_1$ and $\mathbf{r}_2$ are placed on the z axis in such a way that $\mathbf{r}_1 + \mathbf{r}_2 = \mathbf{0}$. From now on, r_{12} will be written as r. We first simplify $G(\mathbf{h}, r)$. According to (76)

$$G(\mathbf{h}, r) = 2\int_0^\infty dz \cos(2\pi z h_z) \int_{\{\mathbf{r}\ |\ z=\text{constant}\}} d^{2n}\mathbf{x}\ f([x^2 + (z + r/2)^2]^{1/2}) e^{2\pi i \mathbf{h}_x\cdot\mathbf{x}} \tag{78}$$

where $x = |\mathbf{x}|$. The integral over the hyperplane $\{\mathbf{r} \mid z = \text{constant}\}$ in (78) has the same form as the integral in (74) if D is replaced by $2n$. It therefore follows from (75) that

$$G(\mathbf{h}, r) = -\frac{2}{h_x^n} \int_0^{1-r/2} dz \cos(2\pi h_z z)[1-(r/2+z)^2]^{n/2} J_n(2\pi h_x [1-(r/2+z)^2]^{1/2}) \quad (79)$$

where $h_x = |\mathbf{h}_x|$. (77) can be rewritten as

$$\chi(r) = \int_{-\infty}^{\infty} dh_z \int_{\mathbf{R}^{2n}} d^{2n}\mathbf{h}_x \; F(h)[G(\mathbf{h}, r)]^2 \quad (80)$$

Since $F(h)$ and $G(\mathbf{h}, r)$ are spherically symmetric in the hyperplane $\{\mathbf{h} \mid h_z = \text{constant}\}$, (80) can be simplified as

$$\chi(r) = \Omega_{2n-1} \int_{-\infty}^{\infty} dh_z \int_0^{\infty} dh_x \; h_x^{2n-1} F(h)[G(\mathbf{h}, r)]^2 \quad (81)$$

where $\Omega_{2n-1} = |S^{2n-1}| = 2\pi^n/\Gamma(n)$. It follows from (75), (79) and (81) that

$$\begin{aligned}\chi(r) = &-\frac{8\pi^n}{\Gamma(n)} \int_0^{1-r/2} dz[1-(r/2+z)^2]^{n/2} \int_0^{1-r/2} dz'[1-(r/2+z')^2]^{n/2} \\ &\int_0^{\infty} dh_x \frac{1}{h_x} J_n\left(2\pi[1-(r/2+z)^2]^{1/2} h_x\right) J_n\left(2\pi[1-(r/2+z')^2]^{1/2} h_x\right) \\ &\int_{-\infty}^{\infty} dh_z \frac{1}{(h_x^2+h_z^2)^{D/4}} J_{D/2}\left(2\pi(h_x^2+h_z^2)^{1/2}\right) \cos(2\pi h_z z) \cos(2\pi h_z z') \quad (82)\end{aligned}$$

We rewrite $\cos(2\pi h_z z)\cos(2\pi h_z z')$ as

$$\cos(2\pi h_z z)\cos(2\pi h_z z') = \frac{1}{2}\{\cos(2\pi h_z(z+z')) + \cos(2\pi h_z(z-z'))\} \quad (83)$$

According to reference [41], p. 772

$$\begin{aligned}&\int_{-\infty}^{\infty} dh_z \frac{1}{(h_x^2+h_z^2)^{D/4}} J_{D/2}\left(2\pi(h_x^2+h_z^2)^{1/2}\right) \cos(2\pi h_z(z \pm z')) \\ &\qquad = \frac{1}{h_x^n}[1-(z \pm z')^2]^{n/2} J_n\left(2\pi h_x[1-(z \pm z')^2]^{1/2}\right) \quad (84)\end{aligned}$$

Thus $\chi(r)$ can be reduced to a three dimensional integral. So

$$\begin{aligned}\chi(r) = \quad &-\frac{4\pi^n}{\Gamma(n)} \int_0^{1-r/2} dz(\alpha(r/2,z)/2\pi)^n \int_0^{1-r/2} dz'(\alpha(r/2,z')/2\pi)^n \\ &\int_0^{\infty} dh_x \frac{1}{{h_x}^{n+1}} J_n(\alpha(r/2,z)h_x) J_n(\alpha(r/2,z')h_x) \\ &\{(\alpha(z,z')/2\pi)^n J_n(\alpha(z,z')h_x) + (\alpha(z,-z')/2\pi)^n J_n(\alpha(z,-z')h_x)\} \quad (85)\end{aligned}$$

where

$$\alpha(z,z') \ = \ 2\pi\sqrt{1-(z+z')^2}. \tag{86}$$

Now we have to evaluate the integral I given by

$$I = \int_0^\infty J_n(\alpha(r/2,z)x)J_n(\alpha(r/2,z')x)J_n(\alpha(z,z')x)\frac{1}{x^{n+1}}dx \tag{87}$$

We integrate by parts and use the recursion relations for Bessel functions

$$J_{\nu-1}(z) + J_{\nu+1}(z) = \frac{2\nu}{z}J_\nu(z) \tag{88}$$

and

$$J_{\nu-1}(z) - J_{\nu+1}(z) = 2\frac{d}{dz}J_\nu(z) \tag{89}$$

Then

$$\begin{aligned} I = \frac{1}{2n} \quad & (\alpha(r/2,z)I_{\alpha(r/2,z);\alpha(r/2,z'),\alpha(z,z')} + \alpha(r/2,z')I_{\alpha(r/2,z');\alpha(r/2,z),\alpha(z,z')} + \\ & +\alpha(z,z')I_{\alpha(z,z');\alpha(r/2,z),\alpha(r/2,z')}) \end{aligned} \tag{90}$$

where

$$I_{\alpha;\beta,\gamma} = \int_0^\infty \frac{1}{x^n}J_{n+1}(\alpha x)J_n(\beta x)J_n(\gamma x)dx \tag{91}$$

and $I_{\beta;\alpha,\gamma}$ and $I_{\gamma;\alpha,\beta}$ are defined as cyclic permutations of the same integral. We use the formula of Sonine and Dougall [45] to calculate $I_{\alpha;\beta,\gamma}$. It says that for any positive constants a, b and c

$$\begin{aligned} & \int_0^\infty J_\mu(at)J_\nu(bt)J_\nu(ct)t^{1-\mu}dt \\ = & \frac{(bc)^\nu 2^{-\mu+1}}{a^\mu\Gamma(\mu-\nu)\Gamma(\nu+1/2)\Gamma(1/2)}\int_0^{A_{a;b,c}}(a^2-b^2-c^2+2bc\cos\varphi)^{\mu-\nu-1}\sin^{2\nu}\varphi\ d\varphi \end{aligned} \tag{92}$$

where

$$A_{a;b,c} = \begin{cases} 0 & \text{if } a^2 < (b-c)^2 \\ \arccos\frac{b^2+c^2-a^2}{2bc} & \text{if } (b-c)^2 < a^2 < (b+c)^2 \\ \pi & \text{if } (b+c)^2 < a^2 \end{cases} \tag{93}$$

Thus

$$I_{\alpha(r/2,z);\alpha(r/2,z'),\alpha(z,z')} = \frac{2^{-n}\alpha(r/2,z')^n\alpha(z,z')^n}{\alpha(r/2,z)^{n+1}\Gamma(n+1/2)\Gamma(1/2)} \int_0^{A_{\alpha(r/2,z);\alpha(r/2,z'),\alpha(z,z')}} \sin^{2n}\varphi \, d\varphi. \tag{94}$$

We have thus reduced $\chi(r)$ to a two dimensional integral:

$$\begin{aligned}
\chi(r) = & -\frac{2\pi^{2n}}{n\Gamma(n+1/2)\Gamma(n)\Gamma(1/2)} \times \\
\times\Bigg(& 2\int_0^{1-r/2} dz \int_0^{1-r/2} dz' (\alpha(r/2,z')/2\pi)^{2n}(\alpha(z,z')/2\pi)^{2n} \\
& \int_0^{A_{\alpha(r/2,z);\alpha(r/2,z'),\alpha(z,z')}} d\varphi \sin^{2n}\varphi \\
+ & \int_0^{1-r/2} dz \int_0^{1-r/2} dz' (\alpha(r/2,z)/2\pi)^{2n}(\alpha(r/2,z')/2\pi)^{2n} \\
& \int_0^{A_{\alpha(z,z');\alpha(r/2,z),\alpha(r/2,z')}} d\varphi \sin^{2n}\varphi \\
+ & \; 2\int_0^{1-r/2} dz \int_0^{1-r/2} dz' (\alpha(r/2,z')/2\pi)^{2n}(\alpha(z,-z')/2\pi)^{2n} \\
& \int_0^{A_{\alpha(r/2,z);\alpha(r/2,z'),\alpha(z,-z')}} d\varphi \sin^{2n}\varphi \\
+ & \int_0^{1-r/2} dz \int_0^{1-r/2} dz' (\alpha(r/2,z)/2\pi)^{2n}(\alpha(r/2,z')/2\pi)^{2n} \\
& \int_0^{A_{\alpha(z,-z');\alpha(r/2,z),\alpha(r/2,z')}} d\varphi \sin^{2n}\varphi \Bigg)
\end{aligned} \tag{95}$$

(The integral over φ may be evaluated using (59).) We need to determine which values of z and z' correspond to which functional form of $A_{a;b,c}$. We will use the fact that for all z, z' for which $0 \le z, z' \le 1 - r/2$

$$\alpha(r/2,z)^2 \le (\alpha(r/2,z') + \alpha(z,z'))^2 \tag{96}$$

and

$$\alpha(z,z')^2 \ge (\alpha(r/2,z) - \alpha(r/2,z'))^2 \tag{97}$$

Since $z' \le 1-r/2 \le r/2$, the first inequality is obvious. The second inequality follows from the first inequality. Since $\alpha(z,-z') \ge \alpha(z,z')$ for all z and z', $\alpha(z,z')$ could be replaced by $\alpha(z,-z')$ in (96) and (97). It follows from (93), (96) and (97) that

$$A_{\alpha(r/2,z);\alpha(r/2,z'),\alpha(z,z')} = \begin{cases} 0 & \text{if } \alpha(r/2,z)^2 < (\alpha(r/2,z') - \alpha(z,z'))^2 \\ \arccos \frac{\alpha(r/2,z')^2+\alpha(z,z')^2-\alpha(r/2,z)^2}{2\alpha(r/2,z)\alpha(z,z')} & \text{if } (\alpha(r/2,z') - \alpha(z,z'))^2 < \alpha(r/2,z)^2 \end{cases} \tag{98}$$

and

$$A_{\alpha(z,z');\alpha(r/2,z),\alpha(r/2,z')} = \begin{cases} \arccos \frac{\alpha(r/2,z)^2+\alpha(r/2,z')^2-\alpha(z,z')^2}{2\alpha(r/2,z)\alpha(r/2,z')} & \text{if } \alpha(z,z')^2 < (\alpha(r/2,z') + \alpha(r/2,z))^2 \\ \pi & \text{if } (\alpha(r/2,z') + \alpha(r/2,z))^2 < \alpha(z,z')^2 \end{cases} \tag{99}$$

We need to translate the equation $\alpha(r/2,z)^2 = (\alpha(r/2,z') - \alpha(z,z'))^2$ into an equation involving z and z'. This can be done by using the definition of α and expanding both sides. In this way it can be shown that

$$A_{\alpha(r/2,z);\alpha(r/2,z'),\alpha(z,z')} = \begin{cases} 0 & \text{if } z' > a_r(z) \\ \arccos \frac{\alpha(r/2,z')^2+\alpha(z,z')^2-\alpha(r/2,z)^2}{2\alpha(r/2,z')\alpha(z,z')} & \text{if } z' < a_r(z) \end{cases} \tag{100}$$

and

$$A_{\alpha(z,z');\alpha(r/2,z),\alpha(r/2,z')} = \begin{cases} \pi & \text{if } z' > a_r(z) \\ \arccos \frac{\alpha(r/2,z)^2+\alpha(r/2,z')^2-\alpha(z,z')^2}{2\alpha(r/2,z)\alpha(r/2,z')} & \text{if } z' < a_r(z) \end{cases} \tag{101}$$

where $z' = a_r(z)$ is the positive root of the equation

$$3 - r^2 - 4z^2 - 4zz' - 4z'^2 - 2rz' + 4r^2zz' + 8rz^2z' + 8rzz'^2 - 2rz = 0. \tag{102}$$

When $r = 1$ this equation can be factorized as

$$(1-2z)(1-2z')(1+z+z') = 0. \tag{103}$$

Hence z' is undetermined whenever $z = 1/2$ in this case.

It can be shown in the same way that

$$A_{\alpha(r/2,z);\alpha(r/2,z'),\alpha(z,-z')} = \begin{cases} 0 & \text{if } z' > b_r(z) \\ \arccos \frac{\alpha(r/2,z')^2+\alpha(z,-z')^2-\alpha(r/2,z)^2}{2\alpha(r/2,z')\alpha(z,-z')} & \text{if } z' < b_r(z) \end{cases} \tag{104}$$

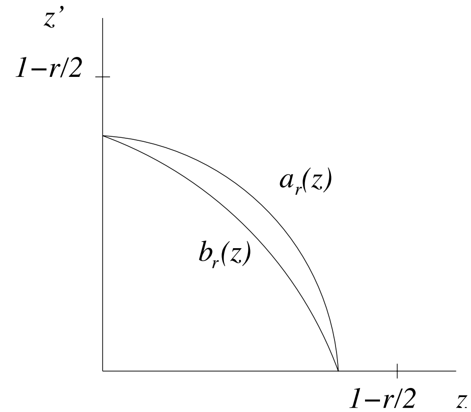


FIG. 1: The functions a_r and b_r. $a_r(z) = b_r(z) = 0$ when $z = -\frac{r}{4} + \frac{1}{4}\sqrt{12 - 3r^2}$.

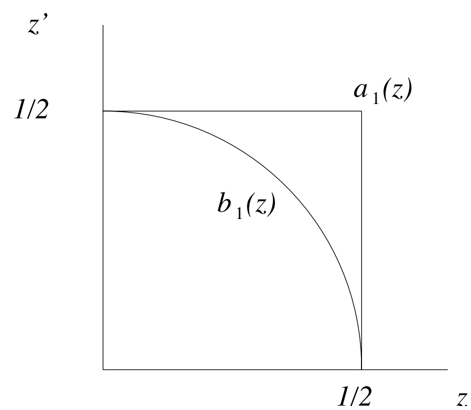


FIG. 2: The functions a_1 and b_1 (here $r = 1$). $b_1(z) = -\frac{1}{4} + \frac{z}{2} + \frac{3}{4}\sqrt{\frac{1}{3}(1-2z)(3+2z)}$. $b_1(z) = 0$ when $z = \frac{1}{2}$.

and

$$A_{\alpha(z,-z');\alpha(r/2,z),\alpha(r/2,z')} = \begin{cases} \pi & \text{if } z' > b_r(z) \\ \arccos \frac{\alpha(r/2,z)^2 + \alpha(r/2,z')^2 - \alpha(z,-z')^2}{2\alpha(r/2,z)\alpha(r/2,z')} & \text{if } z' < b_r(z) \end{cases} \tag{105}$$

where $z' = b_r(z)$ is the positive root of the equation

$$2rz + 2rz' - 4zz' - 3 + 4z^2 + 4z'^2 + r^2 = 0 \tag{106}$$

Since (102) and (106) are both symmetric in z and z', we could equally well write their solutions as $z = a(z')$ and $z = b(z')$ instead. $a_r(z)$ and $b_r(z)$ for $r > 1$ are shown in figure 1.

So

$$
\begin{aligned}
\chi(r) = & - \frac{2\pi^{2n}}{n\Gamma(n+1/2)\Gamma(n)\Gamma(1/2)} \times \\
\times\Bigg(& \quad 2\int_0^{1-r/2} dz \int_0^{a_r(z)} dz'(\alpha(r/2,z')/2\pi)^{2n}(\alpha(z,z')/2\pi)^{2n} \\
& \int_0^{\arccos\left(y_{\alpha(r/2,z);\alpha(r/2,z'),\alpha(z,z')}\right)} d\varphi \ \sin^{2n}\varphi \\
& + \int_0^{1-r/2} dz \int_0^{a_r(z)} dz'(\alpha(r/2,z)/2\pi)^{2n}(\alpha(r/2,z')/2\pi)^{2n} \\
& \int_0^{\arccos\left(y_{\alpha(z,z');\alpha(r/2,z),\alpha(r/2,z')}\right)} d\varphi \ \sin^{2n}\varphi \\
& + 2\int_0^{1-r/2} dz \int_0^{b_r(z)} dz'(\alpha(r/2,z')/2\pi)^{2n}(\alpha(z,-z')/2\pi)^{2n} \\
& \int_0^{\arccos\left(y_{\alpha(r/2,z);\alpha(r/2,z'),\alpha(z,-z')}\right)} d\varphi \ \sin^{2n}\varphi \\
& + \int_0^{1-r/2} dz \int_0^{b_r(z)} dz'(\alpha(r/2,z)/2\pi)^{2n}(\alpha(r/2,z')/2\pi)^{2n} \\
& \int_0^{\arccos\left(y_{\alpha(z,-z');\alpha(r/2,z),\alpha(r/2,z')}\right)} d\varphi \ \sin^{2n}\varphi \\
& + \int_0^{1-r/2} dz \int_{b_r(z)}^{1/2} dz'(\alpha(r/2,z)/2\pi)^{2n}(\alpha(r/2,z')/2\pi)^{2n} \\
& \int_0^{\pi} d\varphi \ \sin^{2n}\varphi \Bigg)
\end{aligned} \tag{107}
$$

where $y_{\alpha;\beta,\gamma} = \frac{\beta^2+\gamma^2-\alpha^2}{2\beta\gamma}$. As r tends to 1, it follows from (103) that $a_r(z)$ takes the value 1/2 for all z, as shown in figure 2. In the special case $r = 1$ the integral simplifies to

$$
\begin{aligned}
\chi(1) = &- \frac{2\pi^{2n}}{n\Gamma(n+1/2)\Gamma(n)\Gamma(1/2)} \times \\
\times\Bigg(\quad & 2\int_0^{1/2} dz \int_0^{1/2} dz' (\alpha(1/2,z')/2\pi)^{2n} (\alpha(z,z')/2\pi)^{2n} \\
& \int_0^{\arccos\left(y_{\alpha(1/2,z);\alpha(1/2,z'),\alpha(z,z')}\right)} d\varphi \ \sin^{2n}\varphi \\
&+ \int_0^{1/2} dz \int_0^{1/2} dz' (\alpha(1/2,z)/2\pi)^{2n} (\alpha(1/2,z')/2\pi)^{2n} \\
& \int_0^{\arccos\left(y_{\alpha(z,z');\alpha(1/2,z),\alpha(1/2,z')}\right)} d\varphi \ \sin^{2n}\varphi \\
&+ 2\int_0^{1/2} dz \int_0^{b_1(z)} dz' (\alpha(1/2,z')/2\pi)^{2n} (\alpha(z,-z')/2\pi)^{2n} \\
& \int_0^{\arccos\left(y_{\alpha(1/2,z);\alpha(1/2,z'),\alpha(z,-z')}\right)} d\varphi \ \sin^{2n}\varphi \\
&+ \int_0^{1/2} dz \int_0^{b_1(z)} dz' (\alpha(1/2,z)/2\pi)^{2n} (\alpha(1/2,z')/2\pi)^{2n} \\
& \int_0^{\arccos\left(y_{\alpha(z,-z');\alpha(1/2,z),\alpha(1/2,z')}\right)} d\varphi \ \sin^{2n}\varphi \\
&+ \int_0^{1/2} dz \int_{b_1(z)}^{1/2} dz' (\alpha(1/2,z)/2\pi)^{2n} (\alpha(1/2,z')/2\pi)^{2n} \\
& \int_0^{\pi} d\varphi \ \sin^{2n}\varphi \Bigg). \qquad (108)
\end{aligned}
$$

After integration by parts, this gives integrals of the type

$$\int \frac{p(x)}{q(x)\sqrt{a+bx+cx^2}} dx, \qquad (109)$$

where p and q are polynomials. Using Maple it was thus possible to calculate $\chi(1)$ for $D = 5, 7, 9, 11$. We may now obtain  from (63). Since  and  can be obtained from (66) and (67), we have found B_4. We use the more compact Ree Hoover $\tilde{f}$ formalism [46] to present the results. In this formalism B_4 consists of only two diagrams instead of three. Here we define a function $\tilde{f}$ by the equation

$$\tilde{f}(r_{ij}) - f(r_{ij}) = 1. \qquad (110)$$

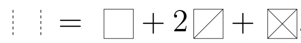
Thus it follows from (6) that $\tilde{f}_{ij} = 0$ precisely when $f_{ij} = -1$. Hence the Mayer complete star has no Ree Hoover bonds, and we write

$\emptyset$ = . (111)

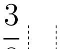
We indicate a Ree Hoover bond by a broken line. The equation

$$\tilde{f}_{14}\tilde{f}_{23} = 1 + f_{14} + f_{23} + f_{14}f_{23} \tag{112}$$

is thus written symbolically as

 (113)

where on the left hand side of (113) only the Ree Hoover bonds are shown. The diagram  is called the Ree Hoover ring, since it consists of a ring of four Mayer bonds and two Ree Hoover bonds. It follows from (10), (111) and (113) that

$$B_4 = \frac{1}{4}\emptyset - \frac{3}{8}$$ . (114)

The final answer is given in tables III, IV and V. For the sake of completeness, we include the diagrams of $B_4^{(3)}$. The numerical values of references [18] and [20] agree with the exact result.

TABLE IV: Exact and numerical [18] values of the Ree Hoover complete star

D	$\frac{\emptyset}{4B_2^3}$	decimal expansion
3	$-\frac{89}{280} - \frac{219}{1120}\frac{\sqrt{2}}{\pi} + \frac{4131}{2240}\frac{\arccos(1/3)}{\pi}$	0.31672598803...
		0.31673(2)
5	$-\frac{163547}{128128} - \frac{3888425}{8200192}\frac{\sqrt{2}}{\pi} + \frac{67183425}{16400384}\frac{\arccos(1/3)}{\pi}$	0.11520591833...
		0.115211(3)
7	$-\frac{283003297}{141892608} - \frac{159966456685}{217947045888}\frac{\sqrt{2}}{\pi} + \frac{292926667005}{48432676864}\frac{\arccos(1/3)}{\pi}$	0.04492254969...
		0.044927(2)
9	$-\frac{88041062201}{34810986496} - \frac{2698457589952103}{2851716013752320}\frac{\sqrt{2}}{\pi} + \frac{8656066770083523}{1140686405500928}\frac{\arccos(1/3)}{\pi}$	0.01828214224...
		0.018286(1)
11	$-\frac{66555106087399}{22760055898112} - \frac{16554115383300832799}{14916030233386680320}\frac{\sqrt{2}}{\pi}$	
	$+\frac{52251492946866520923}{5966412093354672128}\frac{\arccos(1/3)}{\pi}$	0.00766164876...
		0.0076638(8)

TABLE V: Exact and numerical [18] values of the Ree Hoover ring

D	$-\frac{3}{8B_2^3}$	decimal expansion
3	$\frac{4131}{4480}+\frac{657}{2240}\frac{\sqrt{2}}{\pi}-\frac{12393}{4480}\frac{\arccos(1/3)}{\pi}$	$-0.02977648205...$
		$-0.029781(8)$
5	$\frac{67183425}{32800768}+\frac{11665275}{16400384}\frac{\sqrt{2}}{\pi}-\frac{201550275}{32800768}\frac{\arccos(1/3)}{\pi}$	$-0.03923343804...$
		$-0.039233(3)$
7	$\frac{292926667005}{96865353728}+\frac{159966456685}{145298030592}\frac{\sqrt{2}}{\pi}-\frac{878780001015}{96865353728}\frac{\arccos(1/3)}{\pi}$	$-0.03505760307...$
		$-0.035055(3)$
9	$\frac{8656066770083523}{2281372811001856}+\frac{8095372769856309}{5703432027504640}\frac{\sqrt{2}}{\pi}-\frac{25968200310250569}{2281372811001856}\frac{\arccos(1/3)}{\pi}$	$-0.02686294042...$
		$-0.026861(3)$
11	$\frac{5225149294686652092 3}{1193282418670934425 6}$	

D. Theory for the general complete star

We will show that it is possible to construct the complete star of any number of points from some functions F and G. To construct $\chi_{n+2}(r_{12})$ requires n copies of G and $1+2+...+(n-1)=(n-1)n/2$ copies of F. We consider $n+2$ points $\tilde{\mathbf{r}}_1,\ \tilde{\mathbf{r}}_2,\ \mathbf{r}_1, ...,\ \mathbf{r}_n$. We write

$$r=\tilde{r}_{12}:=|\tilde{\mathbf{r}}_1-\tilde{\mathbf{r}}_2|. \tag{115}$$

Let

$$\phi:\{(i,j)\mid 1\le i\le n,\ 1\le j\le n;\ i<j\}\to\{i\mid 1\le i\le n(n-1)/2\} \tag{116}$$

be a bijection, and let

$$\varphi:\{(i,j)\mid 1\le i\le n,\ 1\le j\le n\}\to\{i\mid -n(n-1)/2\le i\le n(n-1)/2\} \tag{117}$$

be an extension of ϕ so that for all (i,j)

$$\varphi(i,j)=-\varphi(j,i). \tag{118}$$

Of course φ is not a bijection. We consider $\mathbf{r} = (\mathbf{x}, z) \in \mathbf{R}^D$ and $\mathbf{h} = (\mathbf{h}_x, h_z) \in \mathbf{R}^{D\star}$ where $\mathbf{R}^{D\star}$ is the dual space of $\mathbf{R}^D$. $\mathbf{R}^{D\star}$ will usually be written as $\mathbf{R}^D$. We use the notation $\mathbf{r}_{(i,j)} := \mathbf{r}_i - \mathbf{r}_j$ and $\mathbf{r}_{-k} := -\mathbf{r}_k$. In particular $\mathbf{r}_{(i,i)} = \mathbf{0}$ and $\mathbf{r}_0 = \mathbf{0}$.

Let

$$f_{(i,j)} := f_{ij}. \tag{119}$$

We define the complete star of $n+2$ points

$$\chi_{n+2}(r) := \prod_{i=1}^{n} \int_{\mathbf{R}^D} d^D\mathbf{r}_i \prod_{j=1}^{n} f_{\tilde{1}j} f_{\tilde{2}j} \prod_{k=1}^{(n-1)n/2} f_{\phi^{-1}(k)}. \tag{120}$$

We proceed by giving some examples. We begin by considering $n = 0$. This is trivial. The integral that needs to be calculated is $\chi_2(r)$. Clearly

$$\chi_2(r) = f_{\tilde{1}\tilde{2}}. \tag{121}$$

In particular,

$$\chi_2(1) = -1. \tag{122}$$

We next consider the case $n = 1$. In this case the integral is

$$\chi_3(r) = \int_{\mathbf{R}^D} f_{\tilde{1}1} f_{\tilde{2}1} d^D\mathbf{r}_1. \tag{123}$$

This integral can be easily evaluated. In particular, when $D = 2$,

$$\chi_3(r) = \int_{r/2}^{1} \sqrt{1-x^2}\, dx \tag{124}$$

and thus

$$\chi_3(1) = \frac{\pi}{3} - \frac{\sqrt{3}}{4}. \tag{125}$$

Our final and only nontrivial examples are $n = 2$ and $n = 3$. It follows from (120) that

$$\chi_4(r) = \int_{\mathbf{R}^D} d^D\mathbf{r}_1 \int_{\mathbf{R}^D} d^D\mathbf{r}_2\; f_{\tilde{1}1} f_{\tilde{2}1} f_{\tilde{1}2} f_{\tilde{2}2} f_{\phi^{-1}(1)}. \tag{126}$$

Following (116), $\phi^{-1}(1)$ can only be $(1,2)$. Thus

$$\chi_4(r) = \int_{\mathbf{R}^D} d^D\mathbf{r}_1 \int_{\mathbf{R}^D} d^D\mathbf{r}_2\; f_{\tilde{1}1} f_{\tilde{2}1} f_{\tilde{1}2} f_{\tilde{2}2} f_{12}. \tag{127}$$

When $n = 3$, ϕ may be chosen so that $\phi(1,2) = 1$, $\phi(1,3) = 2$ and $\phi(2,3) = 3$. Thus

$$\chi_5(r) = \int_{\mathbf{R}^D} d^D\mathbf{r}_1 \int_{\mathbf{R}^D} d^D\mathbf{r}_2 \int_{\mathbf{R}^D} d^D\mathbf{r}_3\; f_{\tilde{1}1} f_{\tilde{2}1} f_{\tilde{1}2} f_{\tilde{2}2} f_{\tilde{1}3} f_{\tilde{2}3} f_{12} f_{13} f_{23}. \tag{128}$$

Lemma 1

$$
\begin{aligned}
\chi_{n+2}(r) = \quad & \prod_{i=1}^{(n-1)n/2} \int_{\mathbf{R}^{D\star}} d^D\mathbf{h}_i \\
& \prod_{j=1}^{n} \int_{\mathbf{R}^D} d^D\mathbf{r}_j \; f_{\tilde{1}j} f_{\tilde{2}j} \exp 2\pi i \sum_{k=1}^{n} \mathbf{h}_{\varphi(j,k)} \cdot (\mathbf{r}_j - \frac{1}{2}(\tilde{\mathbf{r}}_1 + \tilde{\mathbf{r}}_2)) \\
& \prod_{l=1}^{(n-1)n/2} \int_{\mathbf{R}^D} d^D\mathbf{r}'_l \; f_{l'l''} \exp -2\pi i \mathbf{h}_l \cdot (\mathbf{r}'_l - \mathbf{r}''_l)
\end{aligned} \tag{129}
$$

We illustrate the lemma by two examples. For $n = 2$, $\phi : \{(1,2)\} \to \{1\}$, and the right hand side of (129) is

$$
\begin{aligned}
& \int_{\mathbf{R}^{D\star}} d^D\mathbf{h}_1 \int_{\mathbf{R}^D} d^D\mathbf{r}_1 \int_{\mathbf{R}^D} d^D\mathbf{r}_2 \; f_{\tilde{1}1} f_{\tilde{2}1} f_{\tilde{1}2} f_{\tilde{2}2} \exp 2\pi i \mathbf{h}_1 \cdot (\mathbf{r}_1 - \mathbf{r}_2) \\
& \int_{\mathbf{R}^D} d^D\mathbf{r}'_1 \; f_{1'1''} \exp -2\pi i \mathbf{h}_1 \cdot (\mathbf{r}'_1 - \mathbf{r}''_1) \\
= \quad & \int_{\mathbf{R}^D} d^D\mathbf{r}_1 \int_{\mathbf{R}^D} d^D\mathbf{r}_2 \; f_{\tilde{1}1} f_{\tilde{2}1} f_{\tilde{1}2} f_{\tilde{2}2} f_{12} \\
=: \quad & \chi_4(r_{12}).
\end{aligned} \tag{130}
$$

In (130) we used the fact that for an integrable function f continous at $\mathbf{0}$

$$
\int_{\mathbf{R}^D} \int_{\mathbf{R}^D} f(\mathbf{x}) \exp i 2\pi \mathbf{h} \cdot \mathbf{x} \; d^D\mathbf{x} \; d^D\mathbf{h} = f(\mathbf{0}). \tag{131}
$$

From now on, we will assume that the integral $\int_{-\infty}^{\infty} \exp 2\pi i k x \; dk$ exists and equals the Dirac distribution $\delta(x)$. $\delta(x)$ has the property that for any function f continous at 0

$$
\int_{-\infty}^{\infty} \delta(x) f(x) \; dx = f(0). \tag{132}
$$

For $n = 3$, $\phi : \{(1,2),\ (1,3),\ (2,3)\} \to \{1,2,3\}$ and it is easily seen that

$$
\begin{aligned}
& \exp 2\pi i \sum_{j=1}^{n} \sum_{k=1}^{n} \mathbf{h}_{\varphi(j,k)} \cdot (\mathbf{r}_j - \frac{1}{2}(\tilde{\mathbf{r}}_1 + \tilde{\mathbf{r}}_2)) = \\
& \qquad \exp 2\pi i (\mathbf{h}_1 \cdot \mathbf{r}_{\phi^{-1}(1)} + \mathbf{h}_2 \cdot \mathbf{r}_{\phi^{-1}(2)} + \mathbf{h}_3 \cdot \mathbf{r}_{\phi^{-1}(3)}).
\end{aligned} \tag{133}
$$

The general proof is similar to the examples.

Proof of Lemma 1 By changing the order of integration, it is seen that the right hand side of (129) equals

$$\begin{aligned}
& \prod_{i=1}^{n} \int_{\mathbf{R}^D} d^D\mathbf{r}_i \; f_{\tilde{1}i} f_{\tilde{2}i} \prod_{j=1}^{(n-1)n/2} \int_{\mathbf{R}^D} d^D\mathbf{r}'_j \; f_{j'j''} \\
& \prod_{k=1}^{(n-1)n/2} \int_{\mathbf{R}^D} d^D\mathbf{h}_k \prod_{l=1}^{(n-1)n/2} \exp 2\pi i \mathbf{h}_l \cdot (\mathbf{r}''_l - \mathbf{r}'_l + \mathbf{r}_{\phi^{-1}(l)}) \\
= & \prod_{i=1}^{n} \int_{\mathbf{R}^D} d^D\mathbf{r}_i \; f_{\tilde{1}i} f_{\tilde{2}i} \prod_{j=1}^{(n-1)n/2} \int_{\mathbf{R}^D} d^D\mathbf{r}'_j \; f_{j'j''} \prod_{k=1}^{(n-1)n/2} \delta(\mathbf{r}''_k - \mathbf{r}'_k + \mathbf{r}_{\phi^{-1}(k)}) \\
= & \prod_{i=1}^{n} \int_{\mathbf{R}^D} d^D\mathbf{r}_1 \prod_{j=1}^{n} f_{\tilde{1}j} f_{\tilde{2}j} \prod_{k=1}^{(n-1)n/2} f_{\phi^{-1}(k)} \\
=: & \; \chi_{n+2}(r)
\end{aligned} \tag{134}$$

E. Calculation of $\chi_n(r)$ for $D = 2$

Here we will only consider two dimensional hard spheres (in other words, hard disks). This is not very restrictive since a calculation in two dimensions can easily be extended to a calculation in any even dimension. It seems that a calculation in odd dimensions greater than one would be more difficult.

From now on, we let $D = 2$, and we use coordinates $\mathbf{r} = (x, z)$. It follows from (74), (75) and (76) that G can be written as

$$\begin{aligned}
G(\mathbf{h}, r) &= \int_0^{1-r/2} dz \frac{2}{\pi} h_x^{-1} \; \cos 2\pi h_z z \; \sin 2\pi h_x \sqrt{1-(z+r/2)^2} \\
&= 4 \int_0^{1-r/2} dz \cos 2\pi h_z z \int_0^{\sqrt{1-(r/2+z)^2}} dk \; \cos 2\pi h_x k
\end{aligned} \tag{135}$$

From (129) it follows that

$$\chi_{n+2}(r) = \prod_{i=1}^{(n-1)n/2} \int_{\mathbf{R}^{2\star}} d^2\mathbf{h}_i \prod_{k=1}^{n} G\left(\sum_{j=1}^{n} \mathbf{h}_{\varphi(k,j)}, r\right) \prod_{l=1}^{(n-1)n/2} F(\mathbf{h}_l)$$

In particular

$$\chi_4(r) = \int_{\mathbf{R}^{2\star}} d^2\mathbf{h}_1 G\left(\mathbf{h}_1, r\right) G\left(-\mathbf{h}_1, r\right) F(\mathbf{h}_1)$$

and

$$\begin{aligned}
\chi_5(r) = & \int_{\mathbf{R}^{2\star}} d^2\mathbf{h}_1 \int_{\mathbf{R}^{2\star}} d^2\mathbf{h}_2 \int_{\mathbf{R}^{2\star}} d^2\mathbf{h}_3 G\left(\mathbf{h}_1 + \mathbf{h}_2, r\right) G\left(-\mathbf{h}_1 + \mathbf{h}_3, r\right) \\
& G\left(-\mathbf{h}_2 - \mathbf{h}_3, r\right) F(\mathbf{h}_1) F(\mathbf{h}_2) F(\mathbf{h}_3).
\end{aligned} \tag{136}$$

From now on, we let $D = 2$. In light of (75), (135) and (136) it is seen that

$$\chi_{n+2}(r) = (-1)^{(n-1)n/2}4^n \prod_{i=1}^{(n-1)n/2} \int_{\mathbf{R}^{2\star}} d^2\mathbf{h}_i \prod_{j=1}^{n} \int_0^{1-r/2} dz_j \prod_{l=1}^{n} \int_0^{\sqrt{1-(r/2+z_l)^2}} dk_l$$
$$\prod_{p=1}^{n} \cos 2\pi \big(\sum_{q=1}^{n} h_{\varphi(p,q),z} \big) z_p \cos 2\pi \big(\sum_{q=1}^{n} h_{\varphi(p,q),x} \big) k_p$$
$$\prod_{m=1}^{(n-1)n/2} \frac{1}{\left({h_{m,z}}^2 + {h_{m,x}}^2\right)^{1/2}} J_1 \left(2\pi \left({h_{m,z}}^2 + {h_{m,x}}^2\right)^{1/2} \right). \tag{137}$$

In particular

$$\chi_4(r) = -16 \int_{\mathbf{R}^{2\star}} d^2\mathbf{h}_1 \int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \int_0^{\sqrt{1-(r/2+z_1)^2}} dk_1 \int_0^{\sqrt{1-(r/2+z_2)^2}} dk_2$$
$$\cos 2\pi h_{1,z} z_1 \cos(-2\pi h_{1,z} z_2) \cos 2\pi h_{1,x} k_1 \cos(-2\pi h_{1,x} k_2)$$
$$\frac{1}{\left({h_{1,z}}^2 + {h_{1,x}}^2\right)^{1/2}} J_1 \left(2\pi \left({h_{1,z}}^2 + {h_{1,x}}^2\right)^{1/2} \right) \tag{138}$$

and

$$\chi_5(r) = -64 \int_{\mathbf{R}^{2\star}} d^2\mathbf{h}_1 \int_{\mathbf{R}^{2\star}} d^2\mathbf{h}_2 \int_{\mathbf{R}^{2\star}} d^2\mathbf{h}_3 \int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \int_0^{1-r/2} dz_3$$
$$\int_0^{\sqrt{1-(r/2+z_1)^2}} dk_1 \int_0^{\sqrt{1-(r/2+z_2)^2}} dk_2 \int_0^{\sqrt{1-(r/2+z_2)^2}} dk_3$$
$$\cos 2\pi (h_{1,z} + h_{2,z}) z_1 \cos 2\pi (-h_{1,z} + h_{3,z}) z_2 \cos 2\pi (-h_{2,z} - h_{3,z}) z_3$$
$$\cos 2\pi (h_{1,x} + h_{2,x}) k_1 \cos 2\pi (-h_{1,x} + h_{2,x}) k_2 \cos 2\pi (-h_{2,x} - h_{3,x}) k_3$$
$$\frac{1}{\left({h_{1,z}}^2 + {h_{1,x}}^2\right)^{1/2}} J_1 \left(2\pi \left({h_{1,z}}^2 + {h_{1,x}}^2\right)^{1/2} \right)$$
$$\frac{1}{\left({h_{2,z}}^2 + {h_{2,x}}^2\right)^{1/2}} J_1 \left(2\pi \left({h_{2,z}}^2 + {h_{2,x}}^2\right)^{1/2} \right)$$
$$\frac{1}{\left({h_{3,z}}^2 + {h_{3,x}}^2\right)^{1/2}} J_1 \left(2\pi \left({h_{3,z}}^2 + {h_{3,x}}^2\right)^{1/2} \right). \tag{139}$$

We would like to rewrite the product $\prod_{p=1}^{n} \cos 2\pi (\sum_{q=1}^{n} h_{\varphi(p,q),z}) z_p$ in a form that allows us to integrate (137) with respect to $h_z := (h_{1,z}, h_{2,z}, ..., h_{(n-1)n/2,z})$. From now on, we will only use the triple (i, j, p) with the meaning $\phi(i, j) = p$. We will sometimes use the notation $(i_p, j_p, p) = (i, j, \phi(i, j))$.

Lemma 2 Let $\sigma = (\sigma_1, ..., \sigma_{(n-1)n/2}) \in \{-1,\ 1\}^{(n-1)n/2}$. Then the following equality holds under integration:

$$\prod_{i=1}^{n} \cos 2\pi(\sum_{j=1}^{n} h_{\varphi(i,j),z})z_i \equiv \frac{1}{2^{(n-1)n/2}} \sum_{\sigma\in\{-1,1\}^{(n-1)n/2}} \prod_{p=1}^{(n-1)n/2} \cos 2\pi h_{p,z}(z_{i_p} - \sigma_{j_p} z_{j_p}). \tag{140}$$

When $n = 2$, (140) says that

$$\cos 2\pi h_{1,z}z_1 \cos(-2\pi h_{1,z}z_2) \equiv \frac{1}{2}\left(\cos 2\pi h_{1,z}(z_1 - z_2) + \cos 2\pi h_{1,z}(z_1 + z_2)\right). \tag{141}$$

We now illustrate (140) when $n = 3$. In this case, the left hand side of (140) is

$$\cos 2\pi(h_{1,z} + h_{2,z})z_1 \cos 2\pi(-h_{1,z} + h_{3,z})z_2 \cos 2\pi(-h_{2,z} - h_{3,z})z_3 \tag{142}$$

The even part of (142) is

$$\cos h_{1,z}z_1 \cos h_{2,z}z_1 \cos h_{1,z}z_2 \cos h_{3,z}z_2 \cos h_{2,z}z_3 \cos h_{3,z}z_3 + \sin h_{1,z}z_1 \sin h_{2,z}z_1 \sin h_{1,z}z_2 \sin h_{3,z}z_2 \sin h_{2,z}z_3 \sin h_{3,z}z_3. \tag{143}$$

Since $\cos\alpha\cos\beta = (\cos(\alpha-\beta) + \cos(\alpha+\beta))/2$ and $\sin\alpha\sin\beta = (\cos(\alpha-\beta) - \cos(\alpha+\beta))/2$, (143) can be rewritten as

$$\begin{aligned}&\frac{1}{8}(\cos h_{1,z}(z_1 - z_2) + \cos h_{1,z}(z_1 + z_2))(\cos h_{2,z}(z_1 - z_3) + \cos h_{2,z}(z_1 + z_3))\\ &(\cos h_{3,z}(z_2 - z_3) + \cos h_{3,z}(z_2 + z_3)) +\\ &\frac{1}{8}(\cos h_{1,z}(z_1 - z_2) - \cos h_{1,z}(z_1 + z_2))(\cos h_{2,z}(z_1 - z_3) - \cos h_{2,z}(z_1 + z_3))\\ &(\cos h_{3,z}(z_2 - z_3) - \cos h_{3,z}(z_2 + z_3)).\end{aligned} \tag{144}$$

Of course (144) equals (under integration)

$$\begin{aligned}\frac{1}{4}\big(&\cos 2\pi h_{1,z}(z_1 - z_2)\cos 2\pi h_{2,z}(z_1 - z_3)\cos 2\pi h_{3,z}(z_2 - z_3)\\ &+\cos 2\pi h_{1,z}(z_1 - z_2)\cos 2\pi h_{2,z}(z_1 - z_3)\cos 2\pi h_{3,z}(z_2 + z_3)\\ &+\cos 2\pi h_{1,z}(z_1 - z_2)\cos 2\pi h_{2,z}(z_1 + z_3)\cos 2\pi h_{3,z}(z_2 - z_3)\\ &+\cos 2\pi h_{1,z}(z_1 - z_2)\cos 2\pi h_{2,z}(z_1 + z_3)\cos 2\pi h_{3,z}(z_2 + z_3)\big).\end{aligned} \tag{145}$$

(145) is the right hand side of (140) when $n = 3$. The general form clearly follows.

We wish to integrate (140) with respect to $h_z := (h_{1,z}, h_{2,z}, ..., h_{(n-1)n/2,z})$.

It is evident from (140) that $h_{\varphi(i,j),z}$ will appear with a prefactor $(z_i - \sigma_j z_j)$. Stated differently, $h_{p,z}$ will appear with a prefactor $(z_{\phi^{-1}(p)_1} - \sigma_{\phi^{-1}(p)_2} z_{\phi^{-1}(p)_2})$.

We use the formula ([41], p. 772)

$$\int_{-\infty}^{\infty} (x^2+b^2)^{-1/2} J_1(a(x^2+b^2)^{1/2}) \cos cx \; dx$$
$$= \begin{cases} 2a^{-1}b^{-1} \sin b(a^2-c^2)^{1/2} & \text{if } 0 < c < a \\ 0 & \text{if } 0 < a < c. \end{cases} \tag{146}$$

It follows from (137), (140) and (146) that

$$\chi_{n+2}(r) = (-1)^{(n-1)n/2} 4^n \prod_{i=1}^{(n-1)n/2} \int_{-\infty}^{\infty} dh_{i,x} \prod_{j=1}^{n} \int_0^{1-r/2} dz_j \prod_{k=1}^{n} \int_0^{\sqrt{1-(r/2+z_k)^2}} ds_k$$
$$\prod_{l=1}^{n} \cos 2\pi (\sum_{m=1}^{n} h_{\varphi(l,m),x}) s_l$$
$$\frac{1}{2^{(n-1)n/2}} \sum_{\sigma \in \{-1,1\}^{(n-1)n/2}} \prod_{p=1}^{(n-1)n/2} \frac{1}{\pi} \frac{1}{h_{p,x}} \sin 2\pi h_{p,x} \sqrt{1-(z_{i_p} - \sigma_{j_p} z_{j_p})^2}. \tag{147}$$

Using the formula

$$\frac{\sin ax}{x} = \int_0^a \cos xt \; dt \tag{148}$$

(147) can be rewritten as

$$\chi_{n+2}(r) = (-1)^{(n-1)n/2} 4^n \prod_{i=1}^{(n-1)n/2} \int_{-\infty}^{\infty} dh_{i,x} \prod_{j=1}^{n} \int_0^{1-r/2} dz_j \prod_{k=1}^{n} \int_0^{\sqrt{1-(r/2+z_k)^2}} ds_k$$
$$\prod_{l=1}^{n} \cos 2\pi (\sum_{m=1}^{n} h_{\varphi(l,m),x}) s_l$$
$$\sum_{\sigma \in \{-1,1\}^{(n-1)n/2}} \prod_{p=1}^{(n-1)n/2} \int_0^{\sqrt{1-(z_{i_p} - \sigma_{j_p} z_{j_p})^2}} dt_p \; \cos 2\pi h_{p,x} t_p \tag{149}$$

When $n = 2$, this is

$$\chi_4(r) = -16 \int_{-\infty}^{\infty} dh_{1,x} \int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \int_0^{\sqrt{1-(r/2+z_1)^2}} ds_1 \int_0^{\sqrt{1-(r/2+z_2)^2}} ds_2$$
$$\cos 2\pi h_{1,x} s_1 \cos 2\pi - h_{1,x} s_2$$
$$\sum_{\sigma \in \{-1,1\}} \int_0^{\sqrt{1-(z_{i_1} - \sigma_{j_1} z_{j_1})^2}} dt_1 \; \cos 2\pi h_{1,x} t_1 \tag{150}$$

Since in this case $z_{i_1} - \sigma_{j_1} z_{j_1} = z_1 - \sigma z_2$, this is

$$\begin{aligned}\chi_4(r) = \quad & -16 \int_{-\infty}^{\infty} dh_{1,x} \int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \int_0^{\sqrt{1-(r/2+z_1)^2}} ds_1 \int_0^{\sqrt{1-(r/2+z_2)^2}} ds_2 \\ & \cos 2\pi h_{1,x} s_1 \cos(-2\pi h_{1,x} s_2) \\ & \left(\int_0^{\sqrt{1-(z_1-z_2)^2}} + \int_0^{\sqrt{1-(z_1+z_2)^2}} \right) dt_1 \ \cos 2\pi h_{1,x} t_1. \end{aligned} \tag{151}$$

After simplification of the product $\cos 2\pi h_{1,x} s_1 \cos 2\pi h_{1,x} s_2 \cos 2\pi h_{1,x} t_1$, this becomes

$$\begin{aligned}\chi_4(r) = \quad & -4 \int_{-\infty}^{\infty} dh_{1,x} \int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \int_0^{\sqrt{1-(r/2+z_1)^2}} ds_1 \int_0^{\sqrt{1-(r/2+z_2)^2}} ds_2 \\ & \left(\int_0^{\sqrt{1-(z_1-z_2)^2}} + \int_0^{\sqrt{1-(z_1+z_2)^2}} \right) dt_1 \\ & (\cos 2\pi h_{1,x}(s_1 - s_2 - t_1) + \cos 2\pi h_{1,x}(s_1 - s_2 + t_1) + \\ & \cos 2\pi h_{1,x}(s_1 + s_2 - t_1) + \cos 2\pi h_{1,x}(s_1 + s_2 + t_1)). \end{aligned} \tag{152}$$

We may integrate over $h_{1,x}$ to get

$$\begin{aligned}\chi_4(r) = -4 & \int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \int_0^{\sqrt{1-(r/2+z_1)^2}} ds_1 \int_0^{\sqrt{1-(r/2+z_2)^2}} ds_2 \\ & \left(\int_0^{\sqrt{1-(z_1-z_2)^2}} + \int_0^{\sqrt{1-(z_1+z_2)^2}} \right) dt_1 \\ (\delta(s_1 - s_2 - t_1) & + \delta(s_1 - s_2 + t_1) + \delta(s_1 + s_2 - t_1) + \delta(s_1 + s_2 + t_1)). \end{aligned} \tag{153}$$

which becomes

$$\begin{aligned}\chi_4(r) = \quad & -4 \int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \int_0^{\sqrt{1-(r/2+z_1)^2}} ds_1 \int_0^{\sqrt{1-(r/2+z_2)^2}} ds_2 \\ & (\mathbf{1}_{[0<s_1-s_2<\sqrt{1-(z_1-z_2)^2}]} + \mathbf{1}_{[0<s_2-s_1<\sqrt{1-(z_1-z_2)^2}]} \\ & + \mathbf{1}_{[0<s_1+s_2<\sqrt{1-(z_1-z_2)^2}]} + \mathbf{1}_{[0<-s_1-s_2<\sqrt{1-(z_1-z_2)^2}]} \\ & + \mathbf{1}_{[0<s_1-s_2<\sqrt{1-(z_1+z_2)^2}]} + \mathbf{1}_{[0<s_2-s_1<\sqrt{1-(z_1+z_2)^2}]} \\ & + \mathbf{1}_{[0<s_1+s_2<\sqrt{1-(z_1+z_2)^2}]} + \mathbf{1}_{[0<-s_1-s_2<\sqrt{1-(z_1+z_2)^2}]}). \end{aligned} \tag{154}$$

It is clear that

$$\mathbf{1}_{[0<-s_1-s_2<\sqrt{1-(z_1-z_2)^2}]} = \mathbf{1}_{[0<-s_1-s_2<\sqrt{1-(z_1+z_2)^2}]} = 0. \tag{155}$$

Since $1/2 \le r/2 \le \sqrt{3}/2$ and thus $r/2 \le 1 - r/2$, and since $|s_1 - s_2| \le \max\{\sqrt{1-(r/2+z_1)^2}, \sqrt{1-(r/2+z_2)^2}\}$, it is clear that

$$\begin{aligned} & \mathbf{1}_{[0<s_1-s_2<\sqrt{1-(z_1-z_2)^2}]} + \mathbf{1}_{[0<s_2-s_1<\sqrt{1-(z_1-z_2)^2}]} \\ = \; & \mathbf{1}_{[0<s_1-s_2<\sqrt{1-(z_1+z_2)^2}]} + \mathbf{1}_{[0<s_2-s_1<\sqrt{1-(z_1+z_2)^2}]} \\ = \; & 1. \end{aligned} \tag{156}$$

Therefore

$$\begin{aligned} \chi_4(r) = \; & -4 \int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \int_0^{\sqrt{1-(r/2+z_1)^2}} ds_1 \int_0^{\sqrt{1-(r/2+z_2)^2}} ds_2 \\ & (2 + \mathbf{1}_{[0<s_1+s_2<\sqrt{1-(z_1-z_2)^2}]} + \mathbf{1}_{[0<s_1+s_2<\sqrt{1-(z_1+z_2)^2}]}). \end{aligned} \tag{157}$$

Clearly this is

$$\begin{aligned} \chi_4(r) = \; & -4 \int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \\ & (4\alpha\beta - \frac{1}{2}(\alpha+\beta-\gamma)^2 \mathbf{1}_{[\alpha+\beta<\gamma]} - \frac{1}{2}(\alpha+\beta-\delta)^2 \mathbf{1}_{[\alpha+\beta<\delta]}), \end{aligned} \tag{158}$$

where $\alpha := \sqrt{1-(r/2+z_1)^2}$, $\beta := \sqrt{1-(r/2+z_2)^2}$, $\gamma := \sqrt{1-(z_1-z_2)^2}$ and $\delta := \sqrt{1-(z_1+z_2)^2}$. $\chi_4(1)$ can easily be calculated by integration by parts. The equalities

$$\alpha\beta|_{z_2=b_r(z_1)} = \frac{1}{2}(\gamma^2|_{z_2=b_r(z_1)} - \alpha^2 - \beta^2|_{z_2=b_r(z_1)}) \tag{159}$$

and

$$2\arcsin(z - b_r(z)) + \arcsin(r/2 + b_r(z)) = \arcsin(r/2 + z) \tag{160}$$

are useful.

We now consider the case $n = 3$. ϕ may be chosen so that $(i_1, j_1) = (1, 2)$, $(i_2, j_2) = (1, 3)$ and $(i_3, j_3) = (2, 3)$. In this way, (149) is

$$\begin{aligned} \chi_5(r) = \; & \int_{-\infty}^{\infty} dh_{1,x} \int_{-\infty}^{\infty} dh_{2,x} \int_{-\infty}^{\infty} dh_{3,x} \int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \int_0^{1-r/2} dz_3 \\ & \int_0^{\sqrt{1-(r/2+z_1)^2}} ds_1 \int_0^{\sqrt{1-(r/2+z_2)^2}} ds_2 \int_0^{\sqrt{1-(r/2+z_3)^2}} ds_3 \\ & \cos 2\pi(h_{1,x}+h_{2,x})s_1 \cos 2\pi(-h_{1,x}+h_{3,x})s_2 \cos 2\pi(-h_{2,x}-h_{3,x})s_3 \\ & \sum_{\sigma\in\{-1,1\}^3} \int_0^{\sqrt{1-(z_1-\sigma_2 z_2)^2}} dt_1 \int_0^{\sqrt{1-(z_1-\sigma_3 z_3)^2}} dt_2 \int_0^{\sqrt{1-(z_2-\sigma_3 z_3)^2}} dt_3 \\ & \cos 2\pi h_{1,x} t_1 \;\; \cos 2\pi h_{2,x} t_2 \;\; \cos 2\pi h_{3,x} t_3. \end{aligned} \tag{161}$$

Using the representations $\delta(x) = \int_{-\infty}^{\infty} \cos 2\pi kx \ dk$ and $0 = \int_{-\infty}^{\infty} \sin 2\pi kx \ dk$, (161) can be written as

$$\begin{aligned}
\chi_5(r) = \quad & -64 \int_{-\infty}^{\infty} dh_{1,x} \int_{-\infty}^{\infty} dh_{2,x} \int_{-\infty}^{\infty} dh_{3,x} \int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \int_0^{1-r/2} dz_3 \\
& \int_0^{\sqrt{1-(r/2+z_1)^2}} ds_1 \int_0^{\sqrt{1-(r/2+z_2)^2}} ds_2 \int_0^{\sqrt{1-(r/2+z_3)^2}} ds_3 \\
& \sum_{\sigma \in \mathbf{Z}_2^3} \int_0^{\sqrt{1-(\sigma_1 z_1 - \sigma_2 z_2)^2}} dt_1 \int_0^{\sqrt{1-(\sigma_1 z_1 - \sigma_3 z_3)^2}} dt_2 \int_0^{\sqrt{1-(\sigma_2 z_2 - \sigma_3 z_3)^2}} dt_3 \\
& \ \cos 2\pi h_{1,x} t_1 \ \ \cos 2\pi h_{2,x} t_2 \ \ \cos 2\pi h_{3,x} t_3 \\
& \cos 2\pi h_{1,x} s_1 \cos 2\pi h_{1,x} s_2 \cos 2\pi h_{2,x} s_3 \\
& \cos 2\pi h_{2,x} s_1 \cos 2\pi h_{3,x} s_2 \cos 2\pi h_{3,x} s_3. \qquad (162)
\end{aligned}$$

After simplification of the product $\cos 2\pi h_{1,x} s_1 \cos 2\pi h_{1,x} s_2 \cos 2\pi h_{1,x} t_1$, (162) becomes

$$\begin{aligned}
\chi_5(r) = \quad & - \int_{-\infty}^{\infty} dh_{1,x} \int_{-\infty}^{\infty} dh_{2,x} \int_{-\infty}^{\infty} dh_{3,x} \int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \int_0^{1-r/2} dz_3 \\
& \int_0^{\sqrt{1-(r/2+z_1)^2}} ds_1 \int_0^{\sqrt{1-(r/2+z_2)^2}} ds_2 \int_0^{\sqrt{1-(r/2+z_3)^2}} ds_3 \\
& \sum_{\sigma \in \mathbf{Z}_2^3} \int_0^{\sqrt{1-(\sigma_1 z_1 - \sigma_2 z_2)^2}} dt_1 \int_0^{\sqrt{1-(\sigma_1 z_1 - \sigma_3 z_3)^2}} dt_2 \int_0^{\sqrt{1-(\sigma_2 z_2 - \sigma_3 z_3)^2}} dt_3 \\
& \big(\cos 2\pi h_{1,x}(s_1 - s_2 - t_1) + \cos 2\pi h_{1,x}(s_1 - s_2 + t_1) + \\
& \cos 2\pi h_{1,x}(s_1 + s_2 - t_1) + \cos 2\pi h_{1,x}(s_1 + s_2 + t_1) \big) \\
& \big(\cos 2\pi h_{2,x}(s_1 - s_3 - t_2) + \cos 2\pi h_{2,x}(s_1 - s_3 + t_2) + \\
& \cos 2\pi h_{2,x}(s_1 + s_3 - t_2) + \cos 2\pi h_{2,x}(s_1 + s_3 + t_2) \big) \\
& \big(\cos 2\pi h_{3,x}(s_2 - s_3 - t_3) + \cos 2\pi h_{3,x}(s_2 - s_3 + t_3) + \\
& \cos 2\pi h_{3,x}(s_2 + s_3 - t_3) + \cos 2\pi h_{3,x}(s_2 + s_3 + t_3) \big). \qquad (163)
\end{aligned}$$

After integration with respect to h_x, (163) becomes

$$\chi_5(r) = -\int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \int_0^{1-r/2} dz_3$$
$$\int_0^{\sqrt{1-(r/2+z_1)^2}} ds_1 \int_0^{\sqrt{1-(r/2+z_2)^2}} ds_2 \int_0^{\sqrt{1-(r/2+z_3)^2}} ds_3$$
$$\sum_{\sigma\in\mathbf{Z}_2^3} \int_0^{\sqrt{1-(\sigma_1 z_1-\sigma_2 z_2)^2}} dt_1 \int_0^{\sqrt{1-(\sigma_1 z_1-\sigma_3 z_3)^2}} dt_2 \int_0^{\sqrt{1-(\sigma_2 z_2-\sigma_3 z_3)^2}} dt_3$$
$$\big(\delta(s_1-s_2-t_1)+\delta(s_1-s_2+t_1)+\delta(s_1+s_2-t_1)+\delta(s_1+s_2+t_1)\big)$$
$$\big(\delta(s_1-s_3-t_2)+\delta(s_1-s_3+t_2)+\delta(s_1+s_3-t_2)+\delta(s_1+s_3+t_2)\big)$$
$$\big(\delta(s_2-s_3-t_3)+\delta(s_2-s_3+t_3)+\delta(s_2+s_3-t_3)+\delta(s_2+s_3+t_3)\big). \quad (164)$$

Clearly

$$\chi_5(r) = -\int_0^{1-r/2} dz_1 \int_0^{1-r/2} dz_2 \int_0^{1-r/2} dz_3$$
$$\int_0^{\sqrt{1-(r/2+z_1)^2}} ds_1 \int_0^{\sqrt{1-(r/2+z_2)^2}} ds_2 \int_0^{\sqrt{1-(r/2+z_3)^2}} ds_3$$
$$\sum_{\sigma\in\mathbf{Z}_2^3} \big(1+\mathbf{1}_{[s_1+s_2<\sqrt{1-(\sigma_1 z_1-\sigma_2 z_2)^2}]}\big)\big(1+\mathbf{1}_{[s_1+s_3<\sqrt{1-(\sigma_1 z_1-\sigma_3 z_3)^2}]}\big)$$
$$\big(1+\mathbf{1}_{[s_2+s_3<\sqrt{1-(\sigma_2 z_2-\sigma_3 z_3)^2}]}\big). \quad (165)$$

We now consider the general case. We will show that (149) becomes (15). Following Lemma 2, (149) can be rewritten as

$$\chi_{n+2}(r) = (-1)^{(n-1)n/2} 4^n \prod_{i=1}^{(n-1)n/2} \int_{-\infty}^{\infty} dh_{i,x} \prod_{j=1}^{n} \int_0^{1-r/2} dz_j \prod_{k=1}^{n} \int_0^{\sqrt{1-(r/2+z_k)^2}} ds_k$$
$$\frac{1}{2^{n(n-1)/2}} \sum_{\tau\in\{-1,1\}^{(n-1)n/2}} \prod_{q=1}^{n(n-1)/2} \cos 2\pi h_{q,x}(s_{i_q}-\tau_{j_q} s_{j_q})$$
$$\sum_{\sigma\in\{-1,1\}^{(n-1)n/2}} \prod_{p=1}^{(n-1)n/2} \int_0^{\sqrt{1-(z_{i_p}-\sigma_{j_p} z_{j_p})^2}} dt_p \ \cos 2\pi h_{p,x} t_p. \quad (166)$$

Consider the product

$$\prod_{p=1}^{(n-1)n/2} \cos 2\pi h_{p,x}(s_{i_p}-\tau_{j_p} s_{j_p}) \cos 2\pi h_{p,x} t_p. \quad (167)$$

The product (167) can be rewritten as

$$\prod_{p=1}^{(n-1)n/2} \frac{1}{2}(\cos 2\pi h_{p,x}(s_{i_p} - \tau_{j_p} s_{j_p} - t_p) + \cos 2\pi h_{p,x}(s_{i_p} - \tau_{j_p} s_{j_p} + t_p)). \tag{168}$$

The integral over h_x of (168) is

$$\prod_{p=1}^{(n-1)n/2} \frac{1}{2}(\delta(s_{i_p} - \tau_{j_p} s_{j_p} - t_p) + \delta(s_{i_p} - \tau_{j_p} s_{j_p} + t_p)). \tag{169}$$

Therefore (166) becomes

$$\begin{aligned} \chi_{n+2}(r) = \quad & (-1)^{(n-1)n/2} 4^n \prod_{j=1}^{n} \int_0^{1-r/2} dz_j \prod_{k=1}^{n} \int_0^{\sqrt{1-(r/2+z_k)^2}} ds_k \\ & \frac{1}{2^{n(n-1)}} \sum_{\tau \in \{-1,1\}^{(n-1)n/2}} \sum_{\sigma \in \{-1,1\}^{(n-1)n/2}} \\ & \prod_{p=1}^{(n-1)n/2} \Big(\mathbf{1}_{[0 < s_{i_p} - \tau_{j_p} s_{j_p} < \sqrt{1-(z_{i_p} - \sigma_{j_p} z_{j_p})^2}]} + \\ & \mathbf{1}_{[0 < -s_{i_p} + \tau_{j_p} s_{j_p} < \sqrt{1-(z_{i_p} - \sigma_{j_p} z_{j_p})^2}]} \Big). \end{aligned} \tag{170}$$

Executing the sum over τ, (170) becomes

$$\begin{aligned} \chi_{n+2}(r) = \quad & (-1)^{(n-1)n/2} 4^n \prod_{j=1}^{n} \int_0^{1-r/2} dz_j \prod_{k=1}^{n} \int_0^{\sqrt{1-(r/2+z_k)^2}} ds_k \\ & \frac{1}{2^{n(n-1)}} \sum_{\sigma \in \{-1,1\}^{(n-1)n/2}} \\ & \prod_{p=1}^{(n-1)n/2} (\mathbf{1}_{[0 < s_{i_p} - s_{j_p} < \sqrt{1-(z_{i_p} - \sigma_{j_p} z_{j_p})^2}]} + \mathbf{1}_{[0 < s_{i_p} + s_{j_p} < \sqrt{1-(z_{i_p} - \sigma_{j_p} z_{j_p})^2}]} + \\ & \mathbf{1}_{[0 < -s_{i_p} + s_{j_p} < \sqrt{1-(z_{i_p} - \sigma_{j_p} z_{j_p})^2}]} + \mathbf{1}_{[0 < -s_{i_p} - s_{j_p} < \sqrt{1-(z_{i_p} - \sigma_{j_p} z_{j_p})^2}]}). \end{aligned} \tag{171}$$

After simplification, (171) becomes

$$\begin{aligned} \chi_{n+2}(r) = \quad & (-1)^{(n-1)n/2} 4^n \frac{1}{2^{(n-1)n}} \prod_{j=1}^{n} \int_0^{1-r/2} dz_j \prod_{k=1}^{n} \int_0^{\sqrt{1-(r/2+z_k)^2}} ds_k \\ & \sum_{\sigma \in \{-1,1\}^{(n-1)n/2}} \prod_{p=1}^{(n-1)n/2} (1 + \mathbf{1}_{[s_{i_p} + s_{j_p} < \sqrt{1-(z_{i_p} - \sigma_{j_p} z_{j_p})^2}]}). \end{aligned} \tag{172}$$

Thus (15) holds.

TABLE VI: Contributions to the fifth virial coefficient in three dimensions [47], [48]

diagram	exact value
$E5/B_2^4$	$-\frac{40949}{10752}$
$E6\alpha/B_2^4$	$\frac{68419}{26880}$
$E6\beta/B_2^4$	$\frac{82}{35}$
$E7\alpha/B_2^4$	$-\frac{34133}{17920}$
$E7\beta/B_2^4$	$-\frac{18583}{5376}+\frac{33291}{9800}\frac{\sqrt{3}}{\pi}$
$E7\gamma/B_2^4$	$-\frac{73491}{35840}$
$E8\alpha/B_2^4$	unknown
$E8\beta/B_2^4$	$-\frac{35731}{6720}+\frac{1458339}{627200}\frac{\sqrt{2}}{\pi}-\frac{33291}{9800}\frac{\sqrt{3}}{\pi}+\frac{683559}{35840}\frac{\arccos(1/3)}{\pi}$
$E9/B_2^4$	unknown
$E10/B_2^4$	unknown

F. Discussion

Table III shows exact and numerical values of the fourth virial coefficient in dimensions 5, 7, 9 and 11. Typically the relative error of the numerical value is of order 10^{-4}. Recently Clisby and McCoy [18] calculated higher order coefficients using Monte Carlo methods. It is seen that the relative error increases with the order of the coefficient, which is one of the reasons why it is desirable to find analytic values. Table VI shows the known exact values of diagrams of the fifth virial coefficient in 3 dimensions. The diagrams $E7\beta$ and $E8\beta$ have the same coefficient, so there is so far no total contribution of $\sqrt{3}/\pi$. We make the following conjecture:

Conjecture 2 In any dimension, the hard sphere potential (1) allows the analytic computation of every virial coefficient B_n.

No one has so far been able to prove this conjecture. However, since the complete star in odd dimensions can be written in a way similar to equation (15) for 2 dimensions, this conjecture seems plausible.

(15) gives strong support to conjecture 1. One part of $\chi_{n+2}(r)$ is

$$(-1)^{(n-1)n/2}4^n\frac{1}{2^{(n-1)n/2}}\prod_{j=1}^{n}\int_0^{1-r/2}dz_j\prod_{k=1}^{n}\sqrt{1-(r/2+z_k)^2},$$

Following (125), (173) is

$$\frac{(-1)^{(n-1)n/2}}{2^{(n+1)n/2}}(\pi/3 - \sqrt{3}/4)^n,$$

and this number clearly contains all numbers predicted by conjecture 1.

III. THE CORRELATION FUNCTION OF THE TWO DIMENSIONAL ISING LATTICE

A. Introduction

In this chapter, we calculate the correlation functions $\langle \sigma_{0,0}\sigma_{0,N}\rangle$ and $\langle \sigma_{0,0}\sigma_{N,N}\rangle$ as form factor expansions. In section III B, we calculate the exponential expansion of D_N for $T < T_c$, and in section III C we do the same for $T > T_c$. In section III D, we use the result from section III B to calculate D_N as a form factor expansion, and in section III E we use the result from section III C for the same purpose. We conclude in section III F with a discussion.

B. The exponential expansion for $T < T_c$

In this section, we will use the theory of Wiener-Hopf sum equations to prove that the functions $F_N^{(2n)}$ which appear in equation (38) are given by (40).

When $T < T_c$, then $\alpha_1 < \alpha_2 < 1$. In this case we write φ in a factored form as

$$\varphi(z) = P(z)^{-1}Q(z^{-1})^{-1} \tag{173}$$

where the functions $P(z)$ and $Q(z)$ are given by (41) and (42).

When $T < T_c$, then $\alpha_1 < \alpha_2 < 1$ and therefore $P(z)$ and $Q(z)$ are analytic and non-zero for $|z| < 1$. Furthermore the index of φ is

$$\mathrm{Ind}\varphi = \log\varphi(e^{2\pi i}) - \log\varphi(1) = 0 \tag{174}$$

It follows from (174) that we may use Szegö's theorem to find

$$\lim_{N\to\infty} D_N^{(-)} = S_\infty \tag{175}$$

with S_∞ given by (39) which reduces to (24) for both the diagonal and the row correlation functions. Therefore we may write

$$D_N^{(-)} = S_\infty \prod_{n=N}^{\infty} D_n^{(-)}/D_{n+1}^{(-)} \tag{176}$$

1. Computation of the ratio $D_N^{(-)}/D_{N+1}^{(-)}$

The ratio $D_N^{(-)}/D_{N+1}^{(-)}$ is given by

$$D_N^{(-)}/D_{N+1}^{(-)} = x_0^{(N)} \tag{177}$$

where $\mathbf{x}^{(N)} = (x_0, x_1, ..., x_N)$ satisfies

$$\mathbf{A}_{N+1}\mathbf{x}^{(N)} = \mathbf{d}^{(N)} \tag{178}$$

and $d_i^{(N)} = \delta_{i0}$. We indicate that the vector $\mathbf{x}^{(N)}$ has $N+1$ entries by writing $x_0^{(N)}$.

We will calculate $x_0^{(N)}$ by iterating the procedure given by Wu in section 3 of reference [29].

Lemma 1 There are functions $\phi_N^{(2n)}$ such that

$$x_0^{(N)} = 1 + \sum_{n=1}^{\infty} \phi_N^{(2n)} \tag{179}$$

where

$$\begin{aligned} \phi_N^{(2n)} = \; & \frac{(-1)^{n+1}}{(2\pi)^{2n}} \lim_{\epsilon\to 0} \prod_{i=1}^{2n} \oint_{|z_i|=1-\epsilon} dz_i \; z_i^{N+1} \frac{1}{z_1 z_{2n}} \\ & \prod_{k=1}^{n} Q(z_{2k-1}) Q(z_{2k-1}^{-1}) P(z_{2k}) P(z_{2k}^{-1}) \prod_{l=1}^{2n-1} \frac{1}{1 - z_l z_{l+1}}. \end{aligned} \tag{180}$$

Proof Let $h(\xi)$ be a function defined on the unit circle $|\xi| = 1$, and let $h(\xi)$ have the Laurent expansion

$$h(\xi) = \sum_{n=-\infty}^{\infty} h_n \xi^n. \tag{181}$$

From this we define

$$[h(\xi)]_+ = \sum_{n=0}^{\infty} h_n \xi^n, \qquad [h(\xi)]_- = \sum_{n=-\infty}^{-1} h_n \xi^n, \qquad \text{and} \qquad [h(\xi)]'_+ = \sum_{n=1}^{\infty} h_n \xi^n. \tag{182}$$

From equations (182) it follows that

$$[h(\xi^{-1})]_- = [h(\xi)]'_+. \tag{183}$$

Equations (182) have the integral representations

$$[h(\xi)]_+ = \frac{1}{2\pi i} \lim_{\epsilon\to 0} \oint_{|\xi'|=1+\epsilon} d\xi' \frac{h(\xi')}{\xi'-\xi}, \tag{184}$$

$$[h(\xi)]_- = \frac{1}{2\pi i} \lim_{\epsilon\to 0} \oint_{|\xi'|=1-\epsilon} d\xi' \frac{h(\xi')}{\xi-\xi'}, \tag{185}$$

and

$$\begin{aligned}[h(\xi)]'_+ = & \quad [h(\xi)]_+ - \frac{1}{2\pi i} \oint_{|\xi|=1} d\xi \ \frac{h(\xi)}{\xi} \\ = & \quad \frac{1}{2\pi i} \ \xi \lim_{\epsilon\to 0} \oint_{|\xi'|=1+\epsilon} d\xi' \ \frac{h(\xi')}{\xi'(\xi'-\xi)}. \end{aligned} \tag{186}$$

We define

$$X_N(\xi) = \sum_{n=0}^{N-1} x_n^{(N)} \xi^n \tag{187}$$

It has been proven by Wu [29] that the ratio (177) is given by

$$x_0^{(N)} = X_N(0) \tag{188}$$

where $X_N(\xi)$ is a function determined by equations (2.19a)-(2.20b) of reference [29] (with $Y(\xi)=1$). These equations are

$$X_N(\xi) = P(\xi)\left\{[Q(\xi^{-1})]_+ + [Q(\xi^{-1})U_N(\xi)\xi^N]_+\right\} \qquad (2.19\text{a}), \tag{189}$$

$$V_N(\xi^{-1}) = -(Q(\xi^{-1}))^{-1}\left\{[Q(\xi^{-1})]_- + [Q(\xi^{-1})U_N(\xi)\xi^N]_-\right\} \qquad (2.20\text{a}), \tag{190}$$

$$X_N(\xi^{-1})\xi^N = Q(\xi)\left\{[P(\xi^{-1})\xi^N]_+ + [P(\xi^{-1})V_N(\xi)\xi^N]_+\right\} \qquad (2.19\text{b}), \tag{191}$$

and

$$U_N(\xi^{-1}) = -(P(\xi^{-1}))^{-1}\left\{[P(\xi^{-1})\xi^N]_- + [P(\xi^{-1})V_N(\xi)\xi^N]_-\right\} \qquad (2.20\text{b}). \tag{192}$$

For our purposes we use equations (42), (183) and the equality $[Q(\xi^{-1})]_+ = 1$ to rewrite equations (189), (190) and (192) as

$$X_N(\xi) = P(\xi)\left\{1 + [Q(\xi^{-1})U_N(\xi)\xi^N]_+\right\}, \tag{193}$$

$$V_N(\xi^{-1}) = -P(\xi^{-1})\left\{[Q(\xi^{-1})]_- + [Q(\xi^{-1})U_N(\xi)\xi^N]_-\right\}, \tag{194}$$

and

$$U_N(\xi) = -Q(\xi)\left\{[P(\xi)\xi^{-N}]'_+ + [P(\xi)V_N(\xi^{-1})\xi^{-N}]'_+\right\} \tag{195}$$

We define $V_N^{(1)}(\xi^{-1})$ by replacing $U_N(\xi)$ by 0 in equation (194). Thus

$$V_N^{(1)}(\xi^{-1}) = -P(\xi^{-1})[Q(\xi^{-1})]_-. \tag{196}$$

We note from equation (42) that $Q(0) = 1$. Thus, because $Q(\xi^{-1})$ is analytic for $|\xi| > 1$, we have

$$[Q(\xi^{-1})]_- = Q(\xi^{-1}) - Q(0) = Q(\xi^{-1}) - 1. \tag{197}$$

Therefore it follows from equations (42) and (197) that

$$-P(\xi^{-1})[Q(\xi^{-1})]_- = P(\xi^{-1}) - 1, \tag{198}$$

and thus equation (196) becomes

$$V_N^{(1)}(\xi^{-1}) = P(\xi^{-1}) - 1. \tag{199}$$

We define $U_N^{(1)}(\xi)$ by replacing $V_N(\xi^{-1})$ in (195) $V_N^{(1)}(\xi^{-1})$ as given by equation (199). Thus we find

$$U_N^{(1)}(\xi) = -Q(\xi)[P(\xi^{-1})P(\xi)\xi^{-N}]'_+ \tag{200}$$

It follows from equation (193) that $X_N^{(1)}(\xi)$ is given by

$$\begin{aligned} X_N^{(1)}(\xi) &= P(\xi)\Big\{1 - \big[Q(\xi^{-1})Q(\xi)[P(\xi^{-1})P(\xi)\xi^{-N}]'_+\xi^N\big]_+\Big\} \\ &= P(\xi)\Big\{1 - \frac{1}{2\pi i}\lim_{\epsilon\to 0}\oint_{|\xi'|=1+\epsilon} d\xi' \frac{\xi'^N}{\xi' - \xi} \\ &\qquad Q(\xi'^{-1})Q(\xi')[P(\xi'^{-1})P(\xi')\xi'^{-N}]'_+\Big\}. \end{aligned} \tag{201}$$

Letting $\xi = 0$ in equation (201), and using $P(0) = 1$, and writing $X_N^{(1)}(0) = 1 + \phi_N^{(2)}$ we obtain

$$\begin{aligned} \phi_N^{(2)} &= -\frac{1}{2\pi i}\oint_{|\xi|=1} d\xi\; Q(\xi^{-1})Q(\xi)[P(\xi^{-1})P(\xi)\xi^{-N}]'_+\xi^{N-1} \\ &= -\frac{1}{2\pi i}\lim_{\epsilon\to 0}\oint_{|\xi_1|=1} d\xi_1\; Q(\xi_1^{-1})Q(\xi_1)\frac{1}{2\pi i}\xi_1^N \\ &\qquad \oint_{|\xi_2|=1+\epsilon} d\xi_2 \frac{1}{\xi_2}\frac{1}{\xi_2 - \xi_1}P(\xi_2^{-1})P(\xi_2)\xi_2^{-N}. \end{aligned} \tag{202}$$

Thus, if we set

$$\xi_{2k+1} = z_{2k+1}, \qquad \xi_{2k} = z_{2k}^{-1} \tag{203}$$

we obtain $\phi_N^{(2)}$ as given by equation (180).

We now calculate $V_N^{(2)}(\xi^{-1})$ by using equation (200) in equation (194):

$$\begin{aligned} V_N^{(2)}(\xi^{-1}) &= -P(\xi^{-1})\left\{[Q(\xi^{-1})]_- + [Q(\xi^{-1})U_N^{(1)}(\xi)\xi^N]\right\} \\ &= -P(\xi^{-1})[Q(\xi^{-1})]_- \\ &+P(\xi^{-1})\big[Q(\xi^{-1})Q(\xi)\xi^N[P(\xi^{-1})P(\xi)\xi^{-N}]'_+\big]_-. \end{aligned} \tag{204}$$

Next, we calculate $U_N^{(2)}(\xi)$ by using equation (204) in equation (195):

$$\begin{aligned} U_N^{(2)}(\xi) &= -(P(\xi))^{-1}\left\{[P(\xi)\xi^{-N}]'_+ + [P(\xi)V_N^{(2)}(\xi^{-1})\xi^{-N}]'_+\right\} \\ &= -Q(\xi)[P(\xi)P(\xi^{-1})\xi^{-N}]'_+ \\ &-Q(\xi)\Big[P(\xi)P(\xi^{-1})\xi^{-N}\big[Q(\xi)Q(\xi^{-1})\xi^N[P(\xi)P(\xi^{-1})\xi^{-N}]'_+\big]_-\Big]'_+. \end{aligned} \tag{205}$$

We will now calculate $X_N^{(2)}(\xi)$ from (193) and (205) as

$$\begin{aligned} X_N^{(2)}(\xi) &= P(\xi)\{1 + [Q(\xi^{-1})U_N^{(2)}(\xi)\xi^N]_+\} \\ &= P(\xi) - P(\xi)\big[Q(\xi^{-1})Q(\xi)[P(\xi)P(\xi^{-1})\xi^{-N}]'_+\xi^N\big]_+ \\ &-P(\xi)\Big[Q(\xi^{-1})Q(\xi)\xi^N\Big[P(\xi)P(\xi^{-1})\xi^{-N} \\ &\big[Q(\xi)Q(\xi^{-1})\xi^N[P(\xi)P(\xi^{-1})\xi^{-N}]'_+\big]_-\Big]'_+\Big]_+. \end{aligned} \tag{206}$$

Letting $\xi = 0$ in equation (206), we obtain $X_N^{(2)}(0) = 1 + \phi_N^{(2)} + \phi_N^{(4)}$:

$$\begin{aligned} \phi_N^{(4)} &= -\frac{1}{2\pi i}\oint_{|\xi|=1} d\xi\ Q(\xi^{-1})Q(\xi)\Big[P(\xi^{-1})P(\xi)\xi^{-N} \\ &\big[Q(\xi^{-1})Q(\xi)\xi^N[P(\xi^{-1})P(\xi)\xi^{-N}]'_+\big]_-\Big]'_+\xi^{N-1} \\ &= -\frac{1}{(2\pi i)^4}\lim_{\epsilon\to 0}\oint_{|\xi_1|=1} d\xi_1\ \xi_1^N Q(\xi_1^{-1})Q(\xi_1) \\ &\oint_{|\xi_2|=1+\epsilon} d\xi_2\ \frac{1}{\xi_2-\xi_1}\xi_2^{-N-1}P(\xi_2^{-1})P(\xi_2) \\ &\oint_{|\xi_3|=1} d\xi_3\ \frac{1}{\xi_3-\xi_2}\xi_3^{N+1}Q(\xi_3^{-1})Q(\xi_3) \\ &\oint_{|\xi_4|=1+\epsilon} d\xi_4\ \frac{1}{\xi_4-\xi_3}\xi_4^{-N-1}P(\xi_4^{-1})P(\xi_4). \end{aligned} \tag{207}$$

Using the change of variables (203) we obtain an equation agreeing with equation (180).

In general, we iteratively define (from equation 194)

$$V_N^{(n+1)}(\xi^{-1}) = -P(\xi^{-1})\left\{[Q(\xi^{-1})]_- + [Q(\xi^{-1})U_N^{(n)}(\xi)\xi^N]_-\right\}. \tag{208}$$

It then follows from equation (195) that

$$\begin{aligned} U_N^{(n)}(\xi) - U_N^{(n-1)}(\xi) = \quad & -Q(\xi^{-1})\Big[P(\xi)P(\xi^{-1})\xi^{-N}\Big[Q(\xi)Q(\xi^{-1})\xi^N \\ & \big[P(\xi)P(\xi^{-1})\xi^{-N}[Q(\xi)Q(\xi^{-1})\xi^N ...]_-]'_+\big]_-\Big]'_+, \end{aligned} \tag{209}$$

where there are $2n-1$ brackets. It now follows from equations (188) and and (193) that $\phi_N^{(2k)}$ is

$$\begin{aligned} \phi_N^{(2k)} = -\frac{1}{2\pi i}\oint_{|\xi|=1} d\xi\ \xi^{N-1}Q(\xi)Q(\xi^{-1})\Big[P(\xi)P(\xi^{-1})\xi^{-N}\Big[Q(\xi)Q(\xi^{-1})\xi^N \\ \big[P(\xi)P(\xi^{-1})\xi^{-N}[Q(\xi)Q(\xi^{-1})\xi^N ...]_-]'_+\big]_-\Big]'_+, \end{aligned} \tag{210}$$

where there are $2k-1$ brackets. By use of (203), one obtains equation (180). This ends the proof of the lemma.

2. Exponentiation

To complete the proof of the exponential form (38) we need to use (176), (177) and (179) to compute $F_N^{(2n)}$ as given in (40). We begin by defining a function

$$\begin{aligned} \tilde{F}_N^{(2n)} = \quad & \frac{(-1)^{n+1}}{n(2\pi)^{2n}}\lim_{\epsilon\to 0}\prod_{i=1}^{2n}\oint_{|z_i|=1-\epsilon} dz_i \prod_{j=1}^{2n}\frac{z_j^N}{1-z_jz_{j+1}} \\ & \prod_{l=1}^{n} Q(z_{2l-1})Q(z_{2l-1}^{-1})P(z_{2l})P(z_{2l}^{-1})\left(1-\prod_{k=1}^{2n} z_k\right) \end{aligned} \tag{211}$$

(We define $\tilde{F}_N^{(0)} = 0$). Clearly

$$F_N^{(2n)} = \sum_{k=N}^{\infty}\tilde{F}_k^{(2n)}. \tag{212}$$

Let $\phi_N^{(2n)}$ be given by equation (180) when $n \geq 1$ and let $\phi_N^{(0)} = 1$. We define the functions

$$\phi(\lambda) = \sum_{n=0}^{\infty} \phi_N^{(2n)} \lambda^n \tag{213}$$

and

$$\tilde{F}(\lambda) = \sum_{n=0}^{\infty} \tilde{F}_N^{(2n)} \lambda^n. \tag{214}$$

Clearly $\phi(0) = 1$ and $F(0) = 0$. We would like to show that

$$\phi(\lambda) = \exp \tilde{F}(\lambda) \tag{215}$$

It follows as a special case of (215) with $\lambda = 1$ that

$$X_N(0) = \exp \sum_{k=1}^{\infty} \tilde{F}_N^{(2k)}, \tag{216}$$

and hence it follows from equations (176) and (212) that

$$C_N \quad = S_\infty \exp \sum_{k=N}^{\infty} \sum_{n=1}^{\infty} \tilde{F}_k^{(2n)} = S_\infty \exp \sum_{n=1}^{\infty} \sum_{k=N}^{\infty} \tilde{F}_k^{(2n)} = S_\infty \exp \sum_{n=1}^{\infty} F_N^{(2n)} \tag{217}$$

This proves equation (40). It remains to show that equation (215) holds. Since $\phi(0) = 1$ and $F(0) = 0$, equation (215) is equivalent to the equation

$$\phi'(\lambda) = \tilde{F}'(\lambda) \exp \tilde{F}(\lambda) \tag{218}$$

It follows from equations (213), (214) and (218) that equation (215) is equivalent to the following equation:

Lemma 2

$$n\phi_N^{(2n)} = \sum_{l=1}^{n} l \tilde{F}_N^{(2l)} \phi_N^{(2n-2l)}. \tag{219}$$

Proof It follows from (180) that the left hand side of (219) is

$$n\phi_N^{(2n)} = \quad \frac{n(-1)^{n+1}}{(2\pi)^{2n}} \lim_{\epsilon \to 0} \prod_{i=1}^{2n} \oint_{|z_i|=1-\epsilon} dz_i \; z_i^{N+1} \frac{1}{z_{2n} z_1}$$
$$\prod_{j=1}^{n} P(z_{2j}) P(z_{2j}^{-1}) Q(z_{2j-1}) Q(z_{2j-1}^{-1}) \prod_{k=1}^{2n-1} \frac{1}{1 - z_k z_{k+1}}, \tag{220}$$

and the right hand side is

$$\sum_{l=1}^{n} l\tilde{F}_N^{(2l)}\phi_N^{(2n-2l)} = \frac{(-1)^n}{(2\pi)^{2n}}\lim_{\epsilon\to 0}\prod_{i=1}^{2n}\oint_{|z_i|=1-\epsilon} dz_i \prod_{j=1}^{2n}\frac{z_j^N}{1-z_jz_{j+1}}$$
$$\prod_{q=1}^{n} P(z_{2q})P(z_{2q}^{-1})Q(z_{2q-1})Q(z_{2q-1}^{-1})$$
$$\left\{\sum_{l=1}^{n-1}\frac{1}{1-z_1z_{2l}}\left(1-\prod_{k=1}^{2l}z_k\right)(1-z_{2l}z_{2l+1})(1-z_{2n}z_1)\prod_{m=2l+2}^{2n-1}z_m\right.$$
$$\left.-\left(1-\prod_{k=1}^{2n}z_k\right)\right\}, \tag{221}$$

where the product $\prod_{m=2l+2}^{2n-1} z_m$ is such that it equals 1 when $l = n-1$. Note that the product $\prod_{j=1}^{2n}$ is symmetric both in even and in odd variables separately. Hence $1-\prod_{k=1}^{2n} z_k$ can be rewritten (under integration) as

$$1-\prod_{k=1}^{2n} z_k \equiv (1-z_1z_{2n})\left(1+\sum_{q=1}^{n-1}\prod_{r=2}^{2q+1} z_r\right). \tag{222}$$

Next, note that the factor $(1-z_1z_{2l})^{-1}(1-z_{2l}z_{2l+1})(1-z_{2n}z_1)\prod_{m=2l+2}^{2n-1} z_m$ does not involve any of the variables $\{z_i\}_{i=2}^{2l-1}$. Hence the product $1-\prod_{k=1}^{2l} z_k$ can be rewritten as

$$1-\prod_{k=1}^{2l} z_k \equiv (1-z_1z_{2l})\left(1+\sum_{q=1}^{l-1}\prod_{r=2}^{2q+1} z_r\right). \tag{223}$$

Then the relevant factor of the integrand of the right hand side of equation (221) becomes

$$(1-z_{2n}z_1)\left\{\sum_{l=1}^{n-1}(1-z_{2l}z_{2l+1})\left(1+\sum_{q=1}^{l-1}\prod_{r=2}^{2q+1}z_r\right)\prod_{m=2l+2}^{2n-1}z_m-\left(1+\sum_{q=1}^{n-1}\prod_{r=2}^{2q+1}z_r\right)\right\}$$
$$=(1-z_{2n}z_1)\left\{\sum_{l=1}^{n-1}\left(1+\sum_{q=1}^{l-1}\prod_{r=2}^{2q+1}z_r\right)\left(\prod_{m=2l+2}^{2n-1}z_m-\prod_{m=2l}^{2n-1}z_m\right)\right.$$
$$\left.-\left(1+\sum_{q=1}^{n-1}\prod_{r=2}^{2q+1}z_r\right)\right\}. \tag{224}$$

After expansion of the first summand the right hand side of (224) becomes

$$(1-z_{2n}z_1)\left\{\sum_{l=1}^{n-1}\prod_{m=2l+2}^{2n-1}z_m-\sum_{l=1}^{n-1}\prod_{r=2}^{2n-1}z_r-\left(1+\sum_{q=1}^{n-1}\prod_{r=2}^{2q+1}z_r\right)\right\} \tag{225}$$

under integration. After summation (225) becomes

$$-n(1 - z_{2n}z_1)\prod_{r=2}^{2n-1} z_r, \tag{226}$$

which completes the proof. The proof of lemma 2 concludes the proof of equation (40).

C. The exponential expansion for $T > T_c$

In this section, we will prove that the functions $\widehat{F}_N^{(2n)}$ and $G_N^{(2n+1)}$ in (49) are given by (51) and (52). We will follow the procedure of section 2 of Wu [29]. When $T > T_c$, then $\alpha_1 < 1 < \alpha_2$ and $\widehat{\varphi}(z)$ has index 0. We define

$$b_n = \frac{1}{2\pi i}\oint_{|z|=1} \widehat{\varphi}(z) z^{-n-1}\, dz = a_{n-1} \tag{227}$$

We further define

$$\mathbf{B}_{N+1} = \begin{pmatrix} b_0 & b_{-1} & \dots & b_{-N} \\ b_1 & b_0 & \dots & b_{1-N} \\ \vdots & \vdots & \ddots & \vdots \\ b_N & b_{N-1} & \dots & b_0 \end{pmatrix} \tag{228}$$

and

$$\widehat{D}_{N+1} = \det \mathbf{B}_{N+1} \tag{229}$$

We note that if we remove the first row and the last column from $\widehat{D}_{N+1}$ and use (227) we obtain D_N as defined by (32). Therefore we may write

$$D_N^{(+)} = \frac{D_N^{(+)}}{\widehat{D}_{N+1}}\widehat{D}_{N+1} = (-1)^N x_N^{(N)}\widehat{D}_{N+1}, \tag{230}$$

where the ratio $D_N^{(+)}/\widehat{D}_{N+1}$ is given as

$$\frac{D_N^{(+)}}{\widehat{D}_{N+1}} = (-1)^N x_N^{(N)} \tag{231}$$

and $\mathbf{x}^{(N)} = (x_0, x_1, ..., x_N)$ satisfies

$$\mathbf{B}_{N+1}\mathbf{x}^{(N)} = \mathbf{d}^{(N)} \tag{232}$$

and $d_i^{(N)} = \delta_{i0}$. We indicate that the vector $\mathbf{x}^{(N)}$ has $N+1$ entries by writing $x_N^{(N)}$. Since $\widehat{\varphi}(z)$ has index 0, it follows from Szegö's theorem that

$$\lim_{N\to\infty}(-1)^N \widehat{D}_N = \widehat{S}_\infty \tag{233}$$

where $\widehat{S}_\infty$ is given by (50). Thus, exactly as for $T < T_c$,

$$(-1)^{N+1}\widehat{D}_{N+1} = \widehat{S}_\infty \prod_{n=N+1}^{\infty} \frac{\widehat{D}_n}{\widehat{D}_{n+1}}. \tag{234}$$

Furthermore the ratio $\widehat{D}_n/\widehat{D}_{n+1}$ and the product

$$\prod_{n=N+1}^{\infty} \frac{\widehat{D}_n}{\widehat{D}_{n+1}} \tag{235}$$

may be treated exactly as in the case $T < T_c$ if we replace P and Q by $\widehat{P}$ and $\widehat{Q}$. Thus we find

$$(-1)^{N+1}\widehat{D}_{N+1} = \widehat{S}_\infty \exp \sum_{n=1}^{\infty} \widehat{F}_{N+1}^{(2n)}, \tag{236}$$

and hence we have

$$D_N^{(+)} = -\widehat{S}_\infty x_N^{(N)} \exp \sum_{n=1}^{\infty} \widehat{F}_{N+1}^{(2n)}, \tag{237}$$

where we note that when $\alpha_1 = 0$, equation (53) holds.

It remains to calculate $x_N^{(N)}$. We will find $x_N^{(N)}$ by iterating the procedure of section 2 of Wu [29]. We define

$$X_N(\xi) = \sum_{n=0}^{N} x_n^{(N)} \xi^n, \tag{238}$$

and thus

$$x_N^{(N)} = \lim_{\xi\to 0} X_N(\xi^{-1})\xi^N \tag{239}$$

where $X_N(\xi)$ is again defined by (189) to (192) with $P(\xi)$ and $Q(\xi)$ replaced by $\widehat{P}(\xi)$ and $\widehat{Q}(\xi)$. For convenience we rewrite (190), replacing ξ with ξ^{-1} as

$$\begin{aligned} V_N(\xi) &= -\widehat{P}(\xi)\left\{[\widehat{Q}(\xi)]'_+ + [\widehat{Q}(\xi)U_N(\xi^{-1})\xi^{-N}]'_+\right\} \\ &= \widehat{P}(\xi) - 1 - \widehat{P}(\xi)[\widehat{Q}(\xi)U_N(\xi^{-1})\xi^{-N}]'_+. \end{aligned} \tag{240}$$

To obtain the first approximation $x_N^{(N)(1)}$ we replace $U_N(\xi)$ by 0 in (240), and write

$$V_N^{(1)}(\xi) = \widehat{P}(\xi) - 1. \tag{241}$$

We use this in (191) to give

$$X_N^{(1)}(\xi^{-1})\xi^N = \widehat{Q}(\xi)[\widehat{P}(\xi^{-1})\widehat{P}(\xi)\xi^N]_+. \tag{242}$$

Thus, letting ξ approach 0 and using (242) we obtain the first approximation $x_N^{(N)(1)}$, which we denote as $G_N^{(1)}$:

$$G_N^{(1)} = x_N^{(N)(1)} = \frac{1}{2\pi i}\oint_{|\xi|=1} \widehat{P}(\xi^{-1})\widehat{P}(\xi)\xi^{N-1}d\xi. \tag{243}$$

We now compute the second approximation by using (241) in (192) to obtain

$$U_N^{(2)}(\xi^{-1}) = -\widehat{Q}(\xi^{-1})[\widehat{P}(\xi^{-1})\widehat{P}(\xi)\xi^N]_-. \tag{244}$$

We use (244) in (240) to find

$$V_N^{(2)}(\xi) = \widehat{P}(\xi) - 1 + \widehat{P}(\xi)\big[\widehat{Q}(\xi)\widehat{Q}(\xi^{-1})\xi^{-N}[\widehat{P}(\xi^{-1})\widehat{P}(\xi)\xi^N]_-\big]'_+. \tag{245}$$

Using this in (191) we obtain

$$\begin{aligned} X_N^{(2)}(\xi^{-1})\xi^N = \quad & \widehat{Q}(\xi)\Big\{[\widehat{P}(\xi^{-1})\widehat{P}(\xi)\xi^N]_+ \\ & +\Big[\widehat{P}(\xi^{-1})\widehat{P}(\xi)\xi^N\big[\widehat{Q}(\xi^{-1})\widehat{Q}(\xi)\xi^{-N}[\widehat{P}(\xi^{-1})\widehat{P}(\xi)\xi^N]_-\big]'_+\Big]_+\Big\}. \end{aligned} \tag{246}$$

Letting $\xi = 0$ in (246), we see that

$$x_N^{(N)(3)} = G_N^{(1)} + G_N^{(3)}, \tag{247}$$

where

$$\begin{aligned} G_N^{(3)} = \frac{1}{(2\pi i)^3} \quad & \lim_{\epsilon\to 0}\oint_{|z_1|=1} dz_1\; z_1^N\widehat{P}(z_1)\widehat{P}(z_1^{-1})\oint_{|z_2|=1-\epsilon} dz_2\; \frac{z_2^{N+1}}{1-z_1z_2}\widehat{Q}(z_2)\widehat{Q}(z_2^{-1}) \\ & \oint_{|z_3|=1} dz_3\; \frac{z_3^N}{1-z_2z_3}\widehat{P}(z_3)\widehat{P}(z_3^{-1}). \end{aligned} \tag{248}$$

Continuing in the same way we may find

$$x_N^{(N)(2n+1)} = \sum_{k=0}^{n} G_N^{(2k+1)}, \tag{249}$$

and thus

$$D_N^{(+)} = -\widehat{S}_\infty \sum_{n=0}^{\infty} G_N^{(2n+1)} \exp \sum_{m=1}^{\infty} \widehat{F}_{N+1}^{(2m)} \tag{250}$$

where $\widehat{F}_N^{(2n)}$ is defined in (51), $G_N^{(2n+1)}$ is defined in (52) and $\widehat{S}_\infty$ is defined by (50).

If we note that the $G_N^{(2n+1)}$ is the negative of the $G_N^{(2n+1)}$ of [37] and set $\alpha_1 = 0$ we have proven (6) of [37] with $G_N^{(2n+1)}$ given by (34) of [37].

D. The form factor expansion for $T < T_c$

We have showed in section III B that the correlation function $D_N^{(-)}$ can be written in an exponential form given by (38) and (40). In this section we will show that $D_N^{(-)}$ can be written as a form factor expansion given by equations (43) and (6).

We wish to rewrite (38) as a form factor expansion and use an argument similar to that made by Nappi [31] to find the functions $f_N^{(2n)}$. To do this, we denote by a partition π of the number n a set of pairs $\pi = \{(n_i, m_i)\}_{i=1}^{\nu(\pi)}$ such that $n_i \neq n_j$ if $i \neq j$ and

$$\sum_{i=1}^{\nu(\pi)} n_i m_i = n. \tag{251}$$

We define $\mathcal{P}(n)$ to be the set of all such partitions. For instance, the partitions of the number 3 are

$$3 = \begin{cases} 1 \cdot 3, \ \ \nu = 1 \\ 3 \cdot 1, \ \ \nu = 1 \\ 1 \cdot 1 + 2 \cdot 1, \ \ \nu = 2 \ \ . \end{cases} \tag{252}$$

Thus the exponential of (38) may be expanded, and we find

$$f_N^{(2n)} = \sum_{\pi \in \mathcal{P}(n)} \prod_{i=1}^{\nu(\pi)} \frac{1}{m_i!} \left(F_N^{(2n_i)} \right)^{m_i}, \tag{253}$$

where the sum is over the set of partitions $\mathcal{P}(n)$ of the number n. Thus $f_N^{(2n)}$ is the sum of all $2n$ dimensional integrals in (38). Explicitly

$$f_N^{(2n)} = \frac{(-1)^n}{(2\pi)^{2n}} \lim_{\epsilon\to 0} \prod_{i=1}^{2n} \oint_{|z_i|=1-\epsilon} dz_i \; z_i^N \prod_{j=1}^{n} Q(z_{2j-1})Q(z_{2j-1}^{-1})P(z_{2j})P(z_{2j}^{-1}) \frac{1}{1-z_{2j-1}z_{2j}}$$
$$\sum_{\pi\in\mathcal{P}(n)} \prod_{k=1}^{\nu(\pi)} (-1)^{m_k} \frac{1}{m_k! n_k^{m_k}}$$
$$\prod_{p=1}^{m_k} \prod_{q=1}^{n_k} \frac{1}{1 - z_{\sum_{r=1}^{k-1} 2m_r n_r + 2(p-1)n_k + 2q} z_{\sum_{r=1}^{k-1} 2m_r n_r + 2(p-1)n_k + (2q \oplus_{\pi,k} 1)}} \tag{254}$$

where

$$2q \oplus_{\pi,k} 1 = \begin{cases} 2q+1 & \text{if } q < n_k \\ 1 & \text{if } q = n_k. \end{cases} \tag{255}$$

We see that a partition π divides the integrand into $\sum_{k=1}^{\nu(\pi)} m_k$ loops, and that there are m_k loops of length n_k. As an illustration,

$$f_N^{(6)} = -\frac{1}{(2\pi)^6} \lim_{\epsilon\to 0} \prod_{i=1}^{6} \oint_{|z_i|=1-\epsilon} dz_i \; z_i^N \prod_{j=1}^{3} Q(z_{2j-1})Q(z_{2j-1}^{-1})P(z_{2j})P(z_{2j}^{-1})$$
$$\frac{1}{1-z_1z_2}\frac{1}{1-z_3z_4}\frac{1}{1-z_5z_6}$$
$$\Big(-\frac{1}{3!}\frac{1}{1-z_2z_1}\frac{1}{1-z_4z_3}\frac{1}{1-z_6z_5} - \frac{1}{3}\frac{1}{1-z_2z_3}\frac{1}{1-z_4z_5}\frac{1}{1-z_6z_1}$$
$$+\frac{1}{2}\frac{1}{1-z_2z_1}\frac{1}{1-z_4z_5}\frac{1}{1-z_6z_3}\Big) \tag{256}$$

The first term in the bracket of the right hand side of (256) comes from $\pi_1 = \{(1,3)\}$, the second from $\pi_2 = \{(3,1)\}$ and the third from $\pi_3 = \{(1,1),\ (2,1)\}$. We would like to show that

$$f_N^{(2n)} = \frac{1}{n!(2\pi)^{2n}} \lim_{\epsilon\to 0} \prod_{i=1}^{2n} \oint_{|z_i|=1-\epsilon} dz_i \; z_i^N \prod_{j=1}^{n} Q(z_{2j-1})Q(z_{2j-1}^{-1})P(z_{2j})P(z_{2j}^{-1})$$
$$\frac{1}{1-z_{2j-1}z_{2j}} \sum_{\sigma\in S_n} \operatorname{sign}(\sigma) \prod_{k=1}^{n} \frac{1}{1-z_{2k}z_{\sigma(2k-1)}}, \tag{257}$$

where S_n is the group of permutations of the n elements $\{2i-1\}_{i=1}^n$. For instance,

$$S_3 = \{(1)(3)(5),\ (13)(5),\ (15)(3),\ (35)(1),\ (135),\ (153)\} \tag{258}$$

where the loop (abc) means the permutation $a \to b \to c \to a$. We say that two permutations σ_1 and σ_2 in S_n are equivalent if for every loop in σ_1 there is one and only one loop of equal length in σ_2. Then σ_1 and σ_2 will also have the same signature. We write the equivalence class of an element σ as $[\sigma]$. We denote by E_n the set of equivalence classes of S_n. As an example, we have

$$E_3 = \{[(1)(3)(5)],\ [(13)(5)],\ [(135)]\} \tag{259}$$

We will show that there is a bijection between $\mathcal{P}(n)$ and E_n. It is clear that $|\mathcal{P}(3)| = |E_3| = 3$. We will now prove the general case.

We will now calculate $|[\sigma]|$, the number of elements of the equivalence class of a permutation σ. We consider some $\sigma \in S_n$, and construct $[\sigma]$ as follows. We choose freely from n elements, and divide them into $\sum_{i=1}^{\nu} m_i$ loops such that there are m_i loops with n_i elements, without distinguishing between loops with the same number of elements. There are

$$\frac{n!}{\prod_{i=1}^{\nu}(n_i!)^{m_i} m_i!} \tag{260}$$

ways of doing this. There are $(n_i - 1)!$ ways of ordering a loop of n_i elements. Hence, the there are

$$|[\sigma]| = \frac{n! \prod_{i=1}^{\nu}((n_i-1)!)^{m_i}}{\prod_{j=1}^{\nu}(n_j!)^{m_j} m_j!} = \frac{n!}{\prod_{i=1}^{\nu} n_i^{m_i} m_i!} \tag{261}$$

ways of choosing the elements. The signature of any element of the equivalence class $[\sigma]$ corresponding to π is

$$\operatorname{sign}(\sigma) = (-1)^n \prod_{k=1}^{\nu(\pi)} (-1)^{m_k}. \tag{262}$$

If we identify every equivalence class with one of its representatives, then it follows from (254) that

$$\begin{aligned} f_N^{(2n)} = \quad & \frac{1}{n!(2\pi)^{2n}} \lim_{\epsilon \to 0} \prod_{i=1}^{2n} \oint_{|z_i|=1-\epsilon} dz_i\ z_i^N \prod_{j=1}^{n} Q(z_{2j-1}) Q(z_{2j-1}^{-1}) P(z_{2j}) P(z_{2j}^{-1}) \\ & \frac{1}{1 - z_{2j-1} z_{2j}} \sum_{\sigma \in E_n} \operatorname{sign}(\sigma)\ |[\sigma]| \prod_{k=1}^{n} \frac{1}{1 - z_{2k} z_{\sigma(2k-1)}}. \end{aligned} \tag{263}$$

Now (257) follows. By symmetry of the odd variables, (257) can be rewritten as

$$\begin{aligned} f_N^{(2n)} = \quad & \frac{1}{(n!)^2(2\pi)^{2n}} \lim_{\epsilon \to 0} \prod_{i=1}^{2n} \oint_{|z_i|=1-\epsilon} dz_i\ z_i^N \prod_{j=1}^{n} Q(z_{2j-1}) Q(z_{2j-1}^{-1}) P(z_{2j}) P(z_{2j}^{-1}) \\ & \left(\sum_{\sigma \in S_n} \operatorname{sign}(\sigma) \prod_{k=1}^{n} \frac{1}{1 - z_{2k} z_{\sigma(2k-1)}} \right)^2. \end{aligned} \tag{264}$$

Finally we note that the factor of the integrand of (264)

$$\sum_{\sigma\in S_n}\text{sign}(\sigma)\prod_{k=1}^{n}\frac{1}{1-z_{2k}z_{\sigma(2k-1)}} \tag{265}$$

is zero if for any $i\neq j$, $z_{2i}=z_{2j}$ or $z_{2i-1}=z_{2j-1}$. Therefore

$$\sum_{\sigma\in S_n}\text{sign}(\sigma)\prod_{k=1}^{n}\frac{1}{1-z_{2k}z_{\sigma(2k-1)}} = A_n\prod_{k=1}^{n}\prod_{l=1}^{n}\frac{1}{(1-z_{2k-1}z_{2l})} \prod_{1\le p<q\le n}(z_{2p-1}-z_{2q-1})(z_{2p}-z_{2q}). \tag{266}$$

By letting $z_{2n}=z_{2n-1}=0$ we find that

$$A_n=A_{n-1}. \tag{267}$$

Since $A_1=1$, it follows that $A_n=1$ for all n. Hence we obtain the desired result (44).

E. The form factor expansion for $T>T_c$

Above T_c, $D_N^{(+)}$ has a form factor expansion given by (54), where

$$f_N^{(2n+1)}=\sum_{k=0}^{n}G_N^{(2k+1)}\widehat{f}_{N+1}^{(2n-2k)} \tag{268}$$

and $\widehat{f}_N^{(2n)}$ is given by (257) but with P and Q replaced by $\widehat{P}$ and $\widehat{Q}$. $G_N^{(2n+1)}$ is given by (52). Hence it follows from (257), (268) and (52) that

$$\begin{aligned} f_N^{(2n+1)} = & -\frac{i}{(2\pi)^{2n+1}}\lim_{\epsilon\to 0}\prod_{i=1}^{2n+1}\oint_{|z_i|=1-\epsilon}dz_i\; z_i^{N+1}\prod_{l=1}^{n+1}\widehat{P}(z_{2l-1})\widehat{P}(z_{2l-1}^{-1}) \\ & \prod_{m=1}^{n}\widehat{Q}(z_{2m})\widehat{Q}(z_{2m}^{-1})\frac{1}{z_{2n+1}}\prod_{p=1}^{n}\frac{1}{1-z_{2p-1}z_{2p}} \\ & \sum_{k=0}^{n}(-1)^k\frac{1}{(n-k)!}\frac{1}{z_{2n-2k+1}} \\ & \sum_{\sigma\in S_{n-k}}\text{sign}(\sigma)\prod_{q=1}^{n-k}\frac{1}{1-z_{2q-1}z_{\sigma(2q)}}\prod_{s=n-k+1}^{n}\frac{1}{1-z_{2s}z_{2s+1}}. \end{aligned} \tag{269}$$

As an example,

$$\begin{aligned} f_N^{(5)} = & -\frac{i}{(2\pi)^5}\lim_{\epsilon\to 0}\prod_{i=1}^{5}\oint_{|z_i|=1-\epsilon} dz_i \; z_i^{N+1}\prod_{l=1}^{3}\widehat{P}(z_{2l-1})\widehat{P}(z_{2l-1}^{-1}) \\ & \prod_{m=1}^{2}\widehat{Q}(z_{2m})\widehat{Q}(z_{2m}^{-1})\frac{1}{z_5}\frac{1}{1-z_1z_2}\frac{1}{1-z_3z_4} \\ & \left(\frac{1}{2}\frac{1}{z_5}\left(\frac{1}{1-z_1z_2}\frac{1}{1-z_3z_4}-\frac{1}{1-z_1z_4}\frac{1}{1-z_2z_3}\right)\right. \\ & \left.-\frac{1}{z_3}\frac{1}{1-z_1z_2}\frac{1}{1-z_4z_5}+\frac{1}{z_1}\frac{1}{1-z_2z_3}\frac{1}{1-z_4z_5}\right). \end{aligned} \tag{270}$$

Let $(i_1^{(k)},...,i_n^{(k)}) = (1,...,n-k,n-k+2,...,n+1)$. It follows by symmetry that (269) can be rewritten as

$$\begin{aligned} f_N^{(2n+1)} = & -\frac{i}{(2\pi)^{2n+1}}\lim_{\epsilon\to 0}\prod_{i=1}^{2n+1}\oint_{|z_i|=1-\epsilon} dz_i \; z_i^{N+1}\prod_{l=1}^{n+1}\widehat{P}(z_{2l-1})\widehat{P}(z_{2l-1}^{-1}) \\ & \prod_{m=1}^{n}\widehat{Q}(z_{2m})\widehat{Q}(z_{2m}^{-1})\frac{1}{n+1}\sum_{r=0}^{n}(-1)^r\frac{1}{z_{2n-2r+1}}\prod_{p=1}^{n}\frac{1}{1-z_{2i_p^{(r)}-1}z_{2i_p^{(r)}}} \\ & \frac{1}{n!}\sum_{k=0}^{n}(-1)^k\frac{1}{z_{2n-2k+1}}\sum_{\sigma\in S_n}\mathrm{sign}(\sigma)\prod_{q=1}^{n}\frac{1}{1-z_{2i_q^{(k)}-1}z_{\sigma(2i_q^{(k)})}}. \end{aligned} \tag{271}$$

In particular

$$\begin{aligned} f_N^{(5)} = & -\frac{i}{(2\pi)^5}\lim_{\epsilon\to 0}\prod_{i=1}^{5}\oint_{|z_i|=1-\epsilon} dz_i \; z_i^{N+1}\prod_{l=1}^{3}\widehat{P}(z_{2l-1})\widehat{P}(z_{2l-1}^{-1})\prod_{m=1}^{2}\widehat{Q}(z_{2m})\widehat{Q}(z_{2m}^{-1}) \\ & \frac{1}{3}\left(\frac{1}{z_5}\frac{1}{1-z_1z_2}\frac{1}{1-z_3z_4}-\frac{1}{z_3}\frac{1}{1-z_1z_2}\frac{1}{1-z_4z_5}+\frac{1}{z_1}\frac{1}{1-z_2z_3}\frac{1}{1-z_4z_5}\right) \\ & \left\{\frac{1}{2}\frac{1}{z_5}\left(\frac{1}{1-z_1z_2}\frac{1}{1-z_3z_4}-\frac{1}{1-z_1z_4}\frac{1}{1-z_2z_3}\right)\right. \\ & -\frac{1}{2}\frac{1}{z_3}\left(\frac{1}{1-z_1z_2}\frac{1}{1-z_4z_5}-\frac{1}{1-z_1z_4}\frac{1}{1-z_2z_5}\right) \\ & \left.+\frac{1}{2}\frac{1}{z_1}\left(\frac{1}{1-z_2z_3}\frac{1}{1-z_4z_5}-\frac{1}{1-z_3z_4}\frac{1}{1-z_2z_5}\right)\right\}. \end{aligned} \tag{272}$$

Since all permutations of the even elements are present in the sum $\sum_{k=0}^{n}$, symmetry allows the permutation of all even elements in the sum $\sum_{r=0}^{n}$. But the sum $\sum_{k=0}^{n}\sum_{\sigma\in S_n}$

may be rewritten as the sum $\sum_{\sigma\in S_{n+1}}$ of permutations of the odd elements. Therefore

$$f_N^{(2n+1)} = -\frac{i}{(2\pi)^{2n+1}}\lim_{\epsilon\to 0}\prod_{i=1}^{2n+1}\oint_{|z_i|=1-\epsilon} dz_i\ z_i^{N+1}\prod_{l=1}^{n+1}\widehat{P}(z_l)\widehat{P}(z_l^{-1})\prod_{m=1}^{n}\widehat{Q}(z_m)\widehat{Q}(z_m^{-1})$$
$$\frac{1}{n!(n+1)!}\left(\sum_{\sigma\in S_{n+1}}\mathrm{sign}(\sigma)\frac{1}{z_{\sigma(2n+1)}}\prod_{q=1}^{n}\frac{1}{1-z_{\sigma(2q-1)}z_{2q}}\right)^2. \qquad (273)$$

An argument similar to the one given in section III D shows that

$$\sum_{\sigma\in S_{n+1}}\mathrm{sign}(\sigma)\frac{1}{z_{\sigma(2n+1)}}\prod_{q=1}^{n}\frac{1}{1-z_{\sigma(2q-1)}z_{2q}} = \prod_{j=1}^{n+1}\frac{1}{z_{2j-1}}\prod_{k=1}^{n}\frac{1}{1-z_{2j-1}z_{2k}}$$
$$\prod_{1\le l<m\le n+1}(z_{2l-1}-z_{2m-1})\prod_{1\le p<q\le n}(z_{2p}-z_{2q}). \qquad (274)$$

Thus $f_N^{(2n+1)}$ is given by (55) as desired.

F. Discussion

The exponential and the form factor representations derived in this paper for $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ and $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ are considerably simpler that the corresponding representations which may be found in [30]-[34]. The representations of this paper must of course be equal to the corresponding results of [30]-[34] but as mentioned in the introduction even the equality of the form of $F_N^{(2)}$ found by Wu [29] with the form found by Cheng and Wu [26] has not been directly demonstrated in the literature. The form factor representations for $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ proven here are in close correspondence with formulas given by Jimbo and Miwa [49] in their proof of the Painlevé VI representation of the diagonal Ising correlations. The connection which the form factor representations of this paper have with the PVI equation of [49] have been extensively investigated in [37]. However, the representations of this paper are valid also for $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ and, as noted in the introduction, for much more general case which suggests that there are generalizations of [49] which have not yet been uncovered. In particular the relation of $\langle \sigma_{0,0}\sigma_{0,N} \rangle$ to isomonodromic deformation theory remains to be investigated.

---

[1] I. Lyberg: The fourth virial coefficient of a fluid of hard spheres in odd dimensions, J. Stat. Phys., 119, 747, 2005 .

[2] I. Lyberg and B. M. McCoy: Form factor expansion of the row and diagonal correlation functions of the two dimensional Ising model, J. Phys. A, 40, No 13 (2007) 3329.

[3] J. L. Lebowitz and O. Penrose: Convergence of virial expansions, J. Math. Phys. 5 (1964), 841.

[4] J. E. Mayer and M. G. Mayer: *Statistical Mechanics*. Wiley, 1940.

[5] G.E. Uhlenbeck and G. W. Ford, 1962, Studies in Statistical Mechanics, Vol. 1, Ch. 2 (Amsterdam: North-Holland Co.).

[6] J. D. van der Waals: Dissertation, Leiden 1873.

[7] L. Boltzmann: Sitzber. Akad. Wiss. Wien, Math. Natur.-w. Kl. (Pt. 2a) 105, 695, 1896.

[8] G. Jäger: Sitzber. Akad. Wiss. Wien, Math. Natur.-w. Kl. (Pt. 2a) 105, 695, 1896.

[9] J. H. Nairn and J. E. Kilpatrick: van der Waals, Boltzmann, and the fourth virial coefficient of hard spheres. *Am. J. Phys.*, 40:503, 1972.

[10] J.J. van Laar: Berekening der tweede correctie op de grootheid b der toestandsvergli-jjkning van der Waals. *Amsterdam Akad. Versl.*, 7:350-364, 1899.

[11] L. Boltzmann: *Versl. Gewone Vergadering Afk. Natuurk. Nederlandse Akad. Wtensch.*, 7:484, 1899.

[12] B.R.A. Nijboer and L. van Hove: Radial distribution function of a gas of hard spheres and the superposition approximation. *The Physical Review*, Vol. 85, No. 5, 777-783, 1952.

[13] J. de Boer: Reports on Progress in Physics. *Phys. Soc. (London)*, 12, p. 305 (1949).

[14] J.S. Rowlinson: The virial expansion in two dimensions. *Mol. Phys.*, 7:593-594, 1964.

[15] P. C. Hemmer: Virial Coefficients for the Hard-Core Gas in Two Dimensions. *J. Chem. Phys.*, 42:1116-1118, 1965.

[16] N. Clisby and B. M. McCoy: Analytic calculation of B_4 for hard spheres in even dimensions. *J. Stat. Phys.*, Vol. 114, No. 5-6 (2004) 1343.

[17] F. H. Ree and W. G. Hoover: On the signs of the hard sphere virial coefficients. *J. Chem. Phys.*, 40:2048-2049, 1964.

[18] N. Clisby and B. M. McCoy: Negative virial coefficients and the dominance of loose packed diagrams for D-dimensional hard spheres. *J. Stat. Phys.*, Vol. 114, No. 5-6 (2004) 1361.

[19] M. Luban and J. P. J. Michels: Equation of state of hard D-dimensional hyperspheres. *Phys. Rev. A*, 41:6796-6804, 1990.

[20] M. Bishop, A. Masters and J. H. R. Clarke: Equation of state of hard and Weeks-Chandler-Anderson hyperspheres in four and five dimensions. *J. Chem. Phys.*, Vol. 110, No. 23, p. 11449-11453, 1999.

[21] B. Kaufman and L. Onsager, Crystal statistics. III. Short-range order in a binary Ising model, Phys. Rev. 76 (1949) 1244.

[22] E. W. Montroll, R. B. Potts and J. C. Ward, Correlations and spontaneous magnetization of the two dimensional Ising model, J. Math. Phys. 4 (1963) 308.

[23] J. Stephenson, Ising model spin correlations on the triangular latice, J. Math. Phys. 5 (1964) 1009.

[24] K. Yamada, Pair Correlation Function in the Ising Square Lattice - Determinental Form, Prog. Theor. Phys. 72 (1984) 922.

[25] K. Yamada, Pair Correlation Function in the Ising Square Lattice - Generalized Wronskian Form, Prog. Theor. Phys. 76 (1986) 602.

[26] H. Cheng and T.T. Wu, Theory of Toeplitz Determinants and the Spin Correlations of the Two-Dimensional Ising Model. III, Phys. Rev. 162 (1967) 436.

[27] G. Szegö, Commun. Seminair, Math. Univ. Lund, suppl. dédié à Marcel Riesz, 228 (1952).

[28] U. Grenander and G. Szegö, *Toeplitz Forms and their Applications*, University of California Press, Berkeley, 1958.

[29] T. T. Wu, Theory of Toeplitz Determinants and the Spin Correlations of the Two-Dimensional Ising Model, Phys. Rev. 149 (1966) 380.

[30] T. T. Wu, B. M. McCoy, C. A. Tracy and E. Barouch, Spin-spin correlation functions for the two-dimensional Ising model: Exact theory in the scaling region, Phys. Rev. B

13 (1976) 316.

[31] C. R. Nappi, On the Scaling Limit of the Ising Model, Nuovo Cimento A 44 (1978) 392.

[32] J. Palmer and C. Tracy, Two-Dimensional Ising Correlations: Convergence of the Scaling Limit, Adv. Appl. Math. 2 (1981) 329.

[33] B. Nickel, On the singularity of the 2D Ising model susceptibility, J. Phys. A 32 (1999) 3889.

[34] B. Nickel, Addendum to "On the singularity of the 2D Ising model susceptibility", J. Phys. A 33 (2000) 1693.

[35] K. Yamada, On the Spin-Spin Correlation Function in the Ising Square Lattice and the Zero Field Susceptibility, Prog. Theor. Phys. 71 (1984) 1416.

[36] B. M. McCoy and T. T. Wu, *The Two Dimensional Ising Model* (Harvard Univ. Press, Cambridge Mass. 1973) chapters VIII and XI.

[37] S. Boukraa, S. Hassani, J.-M. Maillard, B. M. McCoy, W. P. Orrick and N. Zenine, Holonomy of Ising model form factors, J. Phys. A 40 (2007) 75.

[38] E. Lieb, T. Schultz and D. Mattis, Two soluable models of an antiferromagnetic chain, Ann. Phys. 16 (1961) 407.

[39] B.M. McCoy, Spin correlation functions of the XY model, Phys. Rev. 173 (1968) 531.

[40] E. Barouch and B. McCoy, Statistical mechanics of the XY model II. Spin correlation functions, Phys. Rev, A3 (1971) 786

[41] I. S. Gradshteyn and I. M. Ryzhik: Table of integrals, series and products. *Academic Press, Inc.*, 1994.

[42] J.S. Rowlinson: The triplet distribution function in a fluid of hard spheres. *Mol. Phys.*, 6:517-524, 1963.

[43] M. Luban and A. Baram: Third and fourth virial coefficients of hard hyperspheres of arbitrary dimensionality. *J. Chem. Phys.*, 76:3233-3241, 1982.

[44] C. G. Joslin. Comment on 'Third and fourth virial coefficients of hard hyperspheres of arbitrary dimensionality'. *J. Chem. Phys.*, 77:2701-2702, 1982.

[45] W. Magnus and F. Oberhettinger: Formulas and Theorems for the Functions of Mathematical Physics, p. 37. *Chelsea Publishing Company*, New York 1949.

[46] F. H. Ree and W. G. Hoover: Reformulation of the virial series for classical fluids. *J. Chem. Phys.*, 41:1635-1645, 1964.

[47] S. Kim and D. Henderson: Exact values of two cluster integrals in the fifth virial coefficient for hard spheres. *Physics Letters*, vol. 27A, no. 6, p. 378, 1968.

[48] G. S. Rushbrooke and P. Hutchinson: On the internal consistency of the hyper-chain approximation in the theory of classical fluids. *Physica* 27, p.647, 1961.

[49] M. Jimbo and T. Miwa, Studies on Holonomic Quantum Fields XVII, Proc. Japan Acad. 56A (1980) 405-410;57A (1981) 347.