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One-Dimensional Ising Model in Arbitrary External Field

J. K. Percus[1]

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The external potential needed to produce an arbitrary equilibrium density profile for a one-dimensional lattice gas with nearest neighbor interactions is solved exactly. The resulting sequence of direct correlation functions is shown to be of short range, and in the ferromagnetic case the even members alternate in sign at zero spin. The even Ursell distributions in this case likewise alternate in sign.

KEY WORDS: Ising model; lattice gas; nonuniform; one-dimensional; external field; Ursell distributions; direct correlations.

1. INTRODUCTION

Major progress has been made in recent years toward the elucidation of the structure of bulk systems in classical equilibrium statistical mechanics. Increasing attention is now being paid[1] to the modifying role of spatial inhomogeneity, both for its obvious relevance to the physical world, and as a powerful theoretical tool. An important step in investigations of this kind is the development of exactly solvable model systems, as a check on possible approximations and for the suggestions they may make. One-dimensional models are of course the simplest to derive[2] and can prove very useful, if used with discretion.

In this paper, we shall treat perhaps the simplest nontrivial one-dimensional model, that of an Ising model, or lattice gas with nearest neighbor interactions in an arbitrary external field. We shall proceed by solving the inverse problem of the potential required to evoke a given density profile, and then use standard functional derivative techniques[3] to generate the direct

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[1] Courant Institute of Mathematical Sciences and Physics Department, New York University, New York, New York.

correlation and Ursell correlation sequences. The short-range character of the former will be seen to be maintained in the face of nonuniformity. In addition, a number of positivity properties of both sequences will be established.

2. FORMULATION OF EQUATIONS

The equilibrium statistical mechanics of a lattice gas on the integer lattice $-X \leqslant x \leqslant Y$ is determined by the grand canonical partition function

$$\Xi = \sum_{\{\nu(x)=0,1;-X \leq x \leq Y\}} \exp\left\{-\beta\left[\sum_{-X}^{Y-1} J\nu(x)\nu(x+1) + \sum_{-X}^{Y} u(x)\nu(x)\right]\right\} \quad (1)$$

Here, $u(x)$ is the external potential (including chemical potential), β is the reciprocal temperature, and the interaction has been limited to translation-invariant, nearest neighbor potential with strength J. In this notation, $J < 0$ signifies ferromagnetic interaction. The various distribution functions arise from fixing appropriate summation variables $\nu(x)$, but we will not need more than one to be fixed. Thus, it is convenient to decompose (1) into right and left fragments:

$$R_\nu(x) = \sum_{\{\nu(y)=0,1;x<y\leq Y\}} \exp\{-\beta[J\nu + u(x+1)]\nu(x+1)\} \times \exp\left\{-\beta \sum_{x+2}^{Y} [J\nu(y-1) + u(y)]\nu(y)\right\} \quad (2)$$

$$L_\nu(x) = \sum_{\{\nu(y)=0,1;-X\leq y<x\}} \exp\{-\beta[J\nu + u(x-1)]\nu(x-1)\} \times \exp\left\{-\beta \sum_{-X}^{x-2} [J\nu(y+1) + u(y)]\nu(y)\right\} \quad (3)$$

The principal construct that we shall then need is the lattice density $\rho(x) = \partial(\ln \Xi)/\partial[-\beta u(x)]$, or

$$\rho(x) = (1/\Xi)e^{-\beta u(x)}L_1(x)R_1(x) \quad (4)$$

We will want to take the limit as $X, Y \to \infty$. It is easy to see that $R_\nu(x)$ increases monotonically as Y increases. To ensure convergence, we note that if $J > 0$, $\exp\{-\beta[J\nu + u(y)]\nu(y) \leqslant \exp\{[-\beta u(y)\nu(y)]$. Thus

$$R_\nu(x) \leqslant \sum \prod_{x+1}^{Y} e^{-\beta u(y)\nu(y)} = \prod_{x+1}^{Y} (1 + e^{-\beta u(y)}) \quad (5)$$

converges as long as $\sum_{x+1}^{\infty} e^{-\beta u(y)} < \infty$. Similar considerations apply to $L_\nu(x)$. For $J < 0$, (5) remains valid if we replace $u(y)$ by $J + u(y)$. Hereafter, then, we assume that $X = Y = \infty$. Another consequence of (5) and the corresponding relation for $L_\nu(x)$ is that, since $R_\nu(x), L_\nu(x) \geqslant 1$, we have the boundary conditions

$$R_\nu(\infty) = 1 = L_\nu(-\infty) \tag{6}$$

and then from (1)

$$R_\nu(-\infty) = \Xi = L_\nu(\infty) \tag{7}$$

To examine the properties of $R_\nu(x)$ and $L_\nu(x)$, it is far easier to work with the equations that they satisfy. We have directly from the definitions (2) and (3) the vector relations

$$\begin{pmatrix} R_0(x-1) \\ R_1(x-1) \end{pmatrix} = \begin{pmatrix} 1 & e^{-\beta u(x)} \\ 1 & e^{-\beta J} e^{-\beta u(x)} \end{pmatrix} \begin{pmatrix} R_0(x) \\ R_1(x) \end{pmatrix} \tag{8}$$

$$\begin{pmatrix} L_0(x) \\ L_1(x) \end{pmatrix} = \begin{pmatrix} 1 & e^{-\beta u(x-1)} \\ 1 & e^{-\beta J} e^{-\beta u(x-1)} \end{pmatrix} \begin{pmatrix} L_0(x-1) \\ L_1(x-1) \end{pmatrix} \tag{9}$$

the matrix involved being one of the forms of the usual transfer matrix.[4] Equations (8) and (9), together with (6) or (7), are sufficient in principle to determine $R_\nu(x)$ and $L_\nu(x)$. However, we will not have to write down the full solution—the existence and evaluation of a suitable "constant of motion" will suffice. In general (M^T denoting M-transpose)

$$\begin{aligned} \text{if}\quad & R(x-1) = W(x)R(x), \quad L(x) = U(x)L(x-1), \\ & \text{where } A(x-1)W(x) = U(x)^T A(x), \\ \text{then}\quad & L(x)^T A(x) R(x) = \text{const} \end{aligned} \tag{10}$$

following trivially from $L(x-1)^T A(x-1) R(x-1) = L(x-1)^T A(x-1) W(x)R(x) = L(x-1)^T U(x)^T A(x) R(x) = L^T(x) A(x) R(x)$. In (8) and (9), $U(x) = W(x-1)$ and we may choose

$$A(x) = \begin{pmatrix} 1 & 0 \\ 0 & e^{-\beta u(x)} \end{pmatrix}$$

It follows that $L_0(x)R_0(x) + e^{-\beta u(x)} L_1(x) R_1(x) = \text{const}$. Evaluating the constant by choosing $x \to \pm\infty$, we have

$$L_0(x)R_0(x) + e^{-\beta u(x)} L_1(x) R_1(x) = \Xi \tag{11}$$

Indeed, (11) can be derived directly, in the manner of (4).

3. BASIC SOLUTION

Our primary objective is to find the relation between $u(x)$ and $\rho(x)$. We will do this by eliminating L_0 and R_0 from (11), and then L_1 and R_1 via (4) and a suitable recursion relation for L_1. The process is straightforward. The second components of (8) and (9) read $R_1(x-1) = R_0(x) + e^{-\beta J}e^{-\beta u(x)}R_1(x)$ and $L_1(x) = L_0(x-1) + e^{-\beta J}e^{-\beta u(x-1)}L_1(x-1)$, so that

$$R_0(x) = R_1(x-1) - e^{-\beta J}e^{-\beta u(x)}R_1(x) \tag{12a}$$

$$L_0(x-1) = L_1(x) - e^{-\beta J}e^{-\beta u(x-1)}L_1(x-1) \tag{12b}$$

On the other hand, from the relations inverse to (8) and (9),

$$R(x) = W(x)^{-1}R(x-1), \qquad L(x-1) = W(x-1)^{-1}L(x)$$

$$W(x)^{-1} = \begin{pmatrix} e^{-\beta J}e^{-\beta u(x)} & -e^{-\beta u(x)} \\ -1 & 1 \end{pmatrix} \Big/ e^{-\beta u(x)}(e^{-\beta J} - 1) \tag{13}$$

we have similarly, on taking second components,

$$R_0(x-1) = R_1(x-1) - (e^{-\beta J} - 1)e^{-\beta u(x)}R_1(x) \tag{14a}$$

$$L_0(x) = L_1(x) - (e^{-\beta J} - 1)e^{-\beta u(x-1)}L_1(x-1) \tag{14b}$$

Combining (12) and (14) yields the recursion relations

$$R_1(x-1) - (1 + e^{-\beta J}e^{-\beta u(x)})R_1(x) + (e^{-\beta J} - 1)e^{-\beta u(x+1)}R_1(x+1) = 0 \tag{15a}$$

$$L_1(x+1) - (1 + e^{-\beta J}e^{-\beta u(x)})L_1(x) + (e^{-\beta J} - 1)e^{-\beta u(x-1)}L_1(x-1) = 0 \tag{15b}$$

Let us, in standard notation, set

$$e = e^{-\beta J}, \qquad f = e^{-\beta J} - 1 \tag{16}$$

Eliminating R_0 and L_0 from (11) through (12a) and (14b), we find

$$R_1(x-1)L_1(x) + efe^{-\beta u(x)}e^{-\beta u(x-1)}R_1(x)L_1(x-1)$$
$$- fe^{-\beta u(x-1)}R_1(x-1)L_1(x-1) - fe^{-\beta u(x)}R_1(x)L_1(x) = \Xi$$

and then using (4) to eliminate $R_1(x)$ and $L_1(x-1)$,

$$R_1(x-1)L_1(x) + ef\Xi^2\rho(x)\rho(x-1)/R_1(x-1)L_1(x)$$
$$- f\Xi\rho(x-1) - f\Xi\rho(x) = \Xi$$

Thus, if

$$K(x-1) \equiv (1/\Xi)R_1(x-1)L_1(x) \tag{17}$$

then

$$K(x-1) - [1 + f\rho(x-1) + f\rho(x)] + ef\rho(x)\rho(x-1)/K(x-1) = 0 \tag{18}$$

with the correct root of (18) determined by

$$K(\pm\infty) = 1$$

But from (15b) and (4),

$$e^{-\beta u(x)}K(x)/\rho(x) - (1 + ee^{-\beta u(x)}) + f\rho(x-1)/K(x-1) = 0$$

which may be solved [and simplified by (18), since $K - a + b/K = 0$ implies $b/K - c = a - c - K$, $(K - d)(K + d - a) = d(a - d) - b$] as

$$e^{-\beta u(x)} = \left(f\frac{\rho(x-1)}{K(x-1)} - 1\right)\Big/\left(e - \frac{K(x)}{\rho(x)}\right)$$
$$= \frac{[1 - \rho(x) + f\rho(x-1) - K(x-1)][1 - \rho(x) + f\rho(x+1) - K(x)]}{e^2\rho(x)[1-\rho(x)]} \tag{19}$$

Equations (19) and (18) accomplish the desired end of expressing $u(x)$ in terms of $\rho(x)$. Carrying this out explicitly by solving (18) and substituting into (19), one has

$$e^{-\beta u(x)} = E(\rho(x), \rho(x-1))E(\rho(x), \rho(x+1))/\{4e^2\rho(x)[1-\rho(x)]\} \tag{20}$$

where

$$E(\rho, \rho') \equiv (1 + e)\rho + (1 - e)\rho' - 1 + \{[1 + f(\rho + \rho')]^2 - 4ef\rho\rho'\}^{1/2}$$

Since (20) is a local relation, it is valid independent of the asymptotic requirements associated with (5). This expression can be put in ultimately neater and equally appropriate form by transforming from density to Ising model spin expectation values:

$$\rho(x) \equiv \tfrac{1}{2}(1 + \sigma_x) \tag{21}$$

resulting instead in

$$e^{-\beta u(x)} = F(\sigma_x, \sigma_{x-1})F(\sigma_x, \sigma_{x+1})/[e^2(1 - \sigma_x^2)]$$

where

$$F(\sigma, \sigma') = \tfrac{1}{2}(e + 1)\sigma - \tfrac{1}{2}f\sigma' + \{e + \tfrac{1}{4}f[f\sigma^2 - 2(e + 1)\sigma\sigma' + f\sigma'^2]\}^{1/2} \tag{22}$$

4. DIRECT CORRELATIONS

The successive derivatives of $-\beta u(x)$ with respect to the density at various spatial points are termed the (modified) direct correlation functions. Most heavily studied is the pair direct correlation

$$C(x, y) = \partial[-\beta u(x)]/\partial\rho(y) \tag{23}$$

which must be (and indeed explicitly turns out to be) a symmetric, positive-semidefinite matrix. In the present case, differentiating (20) and transforming by (21), we find that the only nonvanishing matrix elements are given by

$$C(x+1, x) = C(x, x+1) = -f\chi(\sigma_x, \sigma_{x+1})^{-1/2}$$
$$C(x, x) = [1/(1 - \sigma_x^2)]\{[(e + 1) - f\sigma_{x-1}\sigma_x]\chi(\sigma_{x-1}, \sigma_x)^{-1/2} + [(e + 1) - f\sigma_x\sigma_{x+1}]\chi(\sigma_x, \sigma_{x+1})^{-1/2}\} \tag{24}$$

where

$$\chi(\sigma, \sigma') = e + \tfrac{1}{4}f[f\sigma^2 - 2(e + 1)\sigma\sigma' + f\sigma'^2]$$

Thus, $C(x, y)$ has precisely the range $|x - y| \leqslant 1$ of the interaction, as in the uniform case. Further, $C(x, x + 1)$ is everywhere negative or positive as the interaction is ferromagnetic ($J < 0, f > 0$) or antiferromagnetic.

Since C is positive semidefinite, it can be written in various ways in the form

$$C = QQ^T \tag{25}$$

A particularly convenient decomposition is into lower triangular ($y \leqslant x$) and upper triangular factors, and since C has range 1, Q may be taken as of range 1 as well. This assertion follows from the fact that, if assumed true, (25) becomes

$$C(x, x) = Q(x, x)^2 + Q(x, x - 1)^2, \qquad C(x, x + 1) = Q(x, x)Q(x + 1, x) \tag{26}$$

implying that

$$Q(x, x)^2 = C(x, x) - C(x - 1, x)^2/Q(x - 1, x - 1)^2 \tag{27}$$

may be obtained as a continued fraction, which can be shown to converge.[5] The novelty here, perhaps, is that $Q(x, y)$ depends only upon the local density profile. This is most easily seen by noting that, in (24),

$$4\chi(\sigma, \sigma') = [(e + 1) - f\sigma\sigma']^2 - f^2(1 - \sigma^2)(1 - \sigma'^2) \tag{28}$$

and correspondingly rewriting (24) as

$$\begin{aligned} C(x, x) &= \frac{1}{1 - \sigma_x^2}(q_{x-1}^{1/2} + q_{x-1}^{-1/2} + q_x^{1/2} + q_x^{-1/2}) \\ C(x, x + 1) &= -\frac{1}{(1 - \sigma_x^2)^{1/2}(1 - \sigma_{x+1}^2)^{1/2}}(q_x^{1/2} - q_x^{-1/2}) \end{aligned} \tag{29}$$

where

$$q_x = \frac{e + 1 - f\sigma_x\sigma_{x+1} + f(1 - \sigma_x^2)^{1/2}(1 - \sigma_{x+1}^2)^{1/2}}{e + 1 - f\sigma_x\sigma_{x+1} - f(1 - \sigma_x^2)^{1/2}(1 - \sigma_{x+1}^2)^{1/2}}$$

It follows at once that (26) is satisfied by

$$\begin{aligned} Q(x, x) &= \frac{1}{(1 - \sigma_x^2)^{1/2}}(q_x^{1/4} + q_x^{-1/4}) \\ Q(x + 1, x) &= \frac{-1}{(1 - \sigma_{x+1}^2)^{1/2}}(q_x^{1/4} - q_x^{-1/4}) \end{aligned} \tag{30}$$

as required.

We now proceed to the higher direct correlations. These may be defined in general by[3]

$$C_s(x_1, x_2, \ldots, x_s) = \frac{\partial^{s-2} C(x_1, x_2)}{\partial\rho(x_3) \cdots \partial\rho(x_s)} \tag{31}$$

a symmetric function by virtue of (23), and the symmetry of $C(x, y)$. From (24), it follows at once that all C_s are of range 1: They vanish unless $|x_i - x_j| \leqslant 1$ for each pair of arguments. As for their guaranteed signature, let us concentrate on those C_s in which not all arguments are identical. From the short-range property, we can assume that the arguments consist in toto of at least one x and at least one $x + 1$. It is convenient then to define

$$C_{st}(x, x+1) = \frac{\partial^{s-1}}{\partial\rho(x)^{s-1}} \frac{\partial^{t-1}}{\partial\rho(x+1)^{t-1}} C(x, x+1) \tag{32}$$

which, indicating spin density explicitly, means that

$$\sum_{0,0}^{\infty,\infty} \frac{z^{s-1}}{(s-1)!} \frac{w^{t-1}}{(t-1)!} C_{st}(x, x+1) = C(x, x+1 \,|\, \sigma_x + 2z, \sigma_{x+1} + 2w) \tag{33}$$

an appropriate form for investigating properties of the whole sequence.

For a feeling as to what to expect, consider the direct correlations in the uniform spin-symmetric case: $\sigma_x = 0$ for all x of interest. According to (24), the generating function (33) is then given by

$$\begin{aligned} G(z, w) &= -f[e + f(fz^2 - 2(e+1)zw + fw^2)]^{-1/2} \\ &= -f \sum_0^{\infty} (-1)^j \frac{f^j}{e^{j+1/2}} \binom{j - \frac{1}{2}}{j} [fz^2 - 2(e+1)zw + fw^2]^j \end{aligned} \tag{34}$$

C_{st} of course now vanishes if $s + t$ is odd. Suppose $s + t$ is even. Then if $f > 0$ and $z \to iz$, $w \to -iw$, all terms in (34) are negative. On the other hand, for $f < 0$ and $z \to z$, $w \to -w$, all terms in (34) are positive. We conclude from (33) that

$$\text{if} \quad \sigma_x = \sigma_{x+1} = 0 \quad \text{and} \quad s + t \quad \text{is even,} \quad st > 0,$$

$$\text{then} \quad \left.\begin{matrix} (-1)^{(s-t)/2} C_{st}(x, x+1) \\ (-1)^t C_{st}(x, x+1) \end{matrix}\right\} < 0 \quad \text{for} \quad \left\{\begin{matrix} f > 0 \\ f < 0 \end{matrix}\right\} \tag{35}$$

However, (35) does not hold for the general nonuniform lattice. Consider the ferromagnetic case, $f > 0$, with an extreme antiferromagnetic profile, $\sigma_x = 1$, $\sigma_{x+1} = -1$ [this requires a limiting value of the field $u(x)$, which is of no consequence]. Now from (24), (33) becomes

$$G(z, w) = -f\{(e + fz)^2 - 2f[e + (e+1)z]w + f^2 w^2\}^{-1/2} \tag{36}$$

so that

$$G\left(ze, \frac{we}{f}\right) = -\frac{f}{e}\{(1 + fz)^2 - [1 + (e + 1)z]2w + w^2\}^{-1/2}$$

$$= -\frac{f}{e}\sum_0^{\infty} w^n \frac{1}{(1 + fz)^{n+1}} P_n\left(1 + \frac{2z}{1 + fz}\right) \tag{37}$$

where P_n is the nth Legendre polynomial. The w^2z^2 term is typical. Since $P_2(1 + t) = \frac{1}{2}(3t^2 + 6t + 2)$, it becomes

$$w^2z^2: \quad -6(f/e)(f^2 - 4f + 1) \tag{38}$$

and so changes sign in the interval $2 - \sqrt{3} < f < 2 + \sqrt{3}$.

5. URSELL DISTRIBUTIONS

The detailed properties of the lattice gas distributions are most often expressed by means of the cumulants of the microscopic density $\nu(x)$, defined by the generating function[3]

$$\mathscr{F}[w] = \sum_s \frac{(-\beta)^s}{s!} \sum_{x_1,\ldots,x_s} F_s(x_1,\ldots, x_s)w(x_1) \cdots w(x_s)$$

$$= \ln\left\langle \exp\left\{-\beta \sum_x w(x)\nu(x)\right\}\right\rangle \tag{39}$$

For a continuum fluid, the F_s would correspond to the so-called modified Ursell functions. By virtue of (1), $\mathscr{F}[w]$ may be rewritten as

$$\mathscr{F}[w] = \ln(\Xi[u + w]/\Xi[u]) \tag{40}$$

where the external potential in Ξ has been set off in square brackets. It then follows from (39) that for $s \geqslant 1$

$$F_s(x_1,\ldots, x_s) = \frac{\partial^s(\ln \Xi[u])}{\partial\{-\beta u(x_1)\} \cdots \partial\{-\beta u(x_s)\}} \tag{41}$$

The first two of the sequence (41) are of particular importance. Clearly $\rho(x) = \langle\nu(x)\rangle = \partial\mathscr{F}[w]/\partial\{-\beta u(x)\}|_{w=0}$, or

$$\rho(x) = F_1(x) \tag{42}$$

whence

$$F_s(x_1,\ldots, x_s) = \frac{\partial^{s-1}\rho(x_1)}{\partial\{-\beta u(x_2)\} \cdots \partial\{-\beta u(x_s)\}} \tag{43}$$

Further, if S is the matrix inverse to the pair direct correlation of (23), then

$$CS = I \quad \text{or} \quad S(x, y) = \partial\rho(x)/\partial\{-\beta u(y)\} = F_2(x, y) \tag{44}$$

It also follows directly from (39) that

$$S(x, y) = \langle \nu(x)\nu(y)\rangle - \rho(x)\rho(y) = \tfrac{1}{4}(\langle \hat{\sigma}_x \hat{\sigma}_y \rangle - \sigma_x \sigma_y) \tag{45}$$

where $\hat{\sigma}_x \equiv 2\nu(x) - 1$ is the microscopic spin variable, and, as a special case of (45),

$$S(x, x) = \tfrac{1}{4}(1 - \sigma_x{}^2) \tag{46}$$

Let us consider $S(x, y)$ in greater detail. Since $C(x, y)$ is tridiagonal, (44) tells us that $S(x, y)$ satisfies a second-order difference equation. The imposition of boundary conditions as $x \to \pm\infty$ converts this as expected into a first-order equation in each appropriate domain. To see this most directly, we need only rewrite (44), via (25), as

$$Q^T S = Q^{-1} \tag{47}$$

But Q is lower triangular, so Q^{-1} is as well, with reciprocal diagonal elements. Thus we have from (47),

$$\begin{aligned} &\text{if} \quad x \leqslant y, \\ &\text{then} \quad Q(x, x)S(x, y) + Q(x + 1, x)S(x + 1, y) = \frac{1}{Q(x, x)}\,\delta_{x,y} \end{aligned} \tag{48}$$

Indeed, if $x < y$, we have $S(x, y) = -[Q(x + 1, x)/Q(x, x)]S(x + 1, y)$, which iterates at once to the relation

$$x \leqslant y: \quad S(x, y) = \prod_{z=x}^{y-1} [-Q(z + 1, z)/Q(z, z)]S(y, y) \tag{49}$$

Inserting (30) and (46), we thus have

$$x \leqslant y: \quad S(x, y) = \frac{1}{4}(1 - \sigma_x{}^2)^{1/2} \prod_{z=x}^{y-1} \left(\frac{q_z^{1/4} \quad q_z^{-1/4}}{q_z^{1/4} + q_z^{-1/4}}\right)(1 - \sigma_y{}^2)^{1/2} \tag{50}$$

An immediate consequence is that for ferromagnetic coupling, $f \geqslant 0$, $q_x \geqslant 1$, and $S(x, y) \geqslant 0$, whereas in the antiferromagnetic case, $f \leqslant 0$, $q_x \leqslant 1$, $\operatorname{sgn} S(x, y) = (-1)^{y-x}$. An important algebraic consequence of (50) is that

$$\begin{aligned} &\text{if} \quad x \leqslant y \leqslant z \leqslant w, \\ &\text{then} \quad S(x, z)S(y, w) = S(x, w)S(y, z) \end{aligned} \tag{51}$$

To generate the remainder of the sequence F_s, a pivotal role is played by the relation between F_3 and F_2. In order to obtain this, we may first introduce the notation, deriving from (1)–(3),

$$\Xi(x, y) \equiv \sum_{\{\nu(z)=0,1;\, x \leq z \leq y\}} \nu(x)\nu(y)\exp[\beta u(y)] \times \exp\left\{-\beta \sum_{x}^{y-1} [J\nu(z) + u(z + 1)]\nu(z + 1)\right\} \tag{52}$$

for $x \leqslant y$. Direct application of (41) then yields, for $x \leqslant y \leqslant z$,

$$\rho(x) = \Xi(-\infty, x)\Xi(x, \infty)e^{-\beta u(x)}/\Xi$$

$$F_2(x, y) = \Xi(-\infty, x)\Xi(x, y)\Xi(y, \infty)e^{-\beta u(x)}e^{-\beta u(y)}/\Xi - \rho(x)\rho(y) \qquad (53)$$

$$F_3(x, y, z) = \Xi(-\infty, x)\Xi(x, y)\Xi(y, z)\Xi(z, \infty)e^{-\beta u(x)}e^{-\beta u(y)}e^{-\beta u(z)}/\Xi$$
$$- F_2(x, y)\rho(z) - F_2(x, z)\rho(y) - F_2(y, z)\rho(x) - \rho(x)\rho(y)\rho(z)$$

Solving for $\Xi(x, y)$ in terms of $F_2(x, y)$ and substituting into F_3, we have $F_3(x, y, z) = F_2(x, y)F_2(y, z)/\rho(y) - \rho(y)F_2(x, z)$, or, using (51) and (46),

$$F_3(x, y, z) = -\sigma_y F_2(x, z) \qquad (54)$$

Indeed, we can couple (54) with (44), writing them as

$$\frac{\partial F_2(x_1, x_2)}{\partial\{-\beta u(x_3)\}} = -\sigma_{x'} F_2(x_<, x_>), \qquad \frac{\partial \sigma(x_1)}{\partial\{-\beta u(x_2)\}} = 2F_2(x_1, x_2), \qquad (55)$$

where $x_< \leqslant x' \leqslant x_>$. By virtue of

$$F_s(x_1, \ldots, x_s) = \frac{\partial^{s-2}}{\partial\{-\beta u(x_3)\} \cdots \partial\{-\beta u(x_s)\}} F_2(x_1, x_2) \qquad (56)$$

we can thus generate the full sequence of Ursell functions.

Since (55) affords the symbolic replacement $-F_2 \to (-\sigma)(-F_2)$, $-\sigma \to -F_2$, (56) creates the general form[6]

$$F_s = -P\{-F_2, -\sigma\} \qquad (57)$$

where P is a polynomial each of whose monomial terms has positive sign, weight s with σ of weight 1, F_2 of weight 2, and has each argument present just once. If $f > 0$, then $F_2 \geqslant 0$, and if $\sigma = 0$ throughout, F_{2s} being of degree s in the F_2 implies that

$$f > 0, \sigma = 0; \quad \operatorname{sgn}(F_{2s}) = (-1)^{s+1} \qquad (58)$$

(in contrast to the continuum fluid F_s with repulsive forces[7]). This has been proven by Rosen[8] and F_{2s} is exhibited in very explicit form. However, the generalization to arbitrary external field does not hold. It is only necessary to look at F_4 to see this. According to (55) and (56),

$$x \leqslant y \leqslant z \leqslant w\colon \quad F_4(x, y, z, w) = -F_2(x, w)[2F_2(y, z) - \sigma(y)\sigma(z)] \qquad (59)$$

and there is no difficulty in rendering this expression positive by selecting small $F_2(x, w)$, $F_2(y, z)$.

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