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The Nonuniform Hard-Rod Fluid Revisited

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The statistical mechanics of the one-dimensional nonuniform pure hard-core fluid is formulated in the spirit of the Reiss–Frisch–Lebowitz (RFL) scaled particle theory. By emphasizing the importance of the core dependence, a more intuitive and simpler derivation can be given. The Wiener–Hopf-type construction of the pair direct correlation function is formulated via the Dyson variational method of inverse scattering theory, which is compared with the particle–hole theory. The new approach allows us to lift the global free energy functional into a larger space where all the symmetries become apparent.

KEY WORDS: Hard-rod fluid; nonuniform; variational principle; Wiener–Hopf factorization; scaled particle theory.

1. INTRODUCTION

The study of the structure of nonuniform fluids has attracted more and more attention (see, e.g., ref. 1). Much of the progress has relied upon the knowledge of hard-core fluids, just as had been the case for uniform fluids. As in any other field, exactly solvable models are rare. But once they are found, there will be profound impact on our understanding, which will help us to create more effective approximation schemes. One such example is the classical hard-rod fluid in an external field. The exact solution was given by Percus[2] in 1976 using density functional theory, and the corresponding discrete version was solved by Robledo[3] in 1979 using potential distribution theory. These results were used to produce better approximate solutions for higher-dimensional models[3,4] and mixtures.[5]

In this paper, we would like to reexamine the model from a different viewpoint in order to fully appreciate the beauty of the model and firmly grasp the physical content of the solution. Therefore, this paper may be

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regarded as complementary to refs. 2 and 3. In Section 2, we start with the corresponding discrete model, derive a pair of "characteristic equations," and use it to find the (inverse) profile equation. In Section 3, we obtain the continuum limit by introducing local pressure fields. In Section 4, we reverse the logic and present a simple physical approach by RFL scaled-particle-type reasoning. In Section 5, we point out the relation between the Wiener–Hopf factorization of the pair direct correlation function and the Dyson variational method in the inverse scattering theory of quantum mechanics, and compare the latter with particle–hole theory. In the last section, we push the idea further to lift the global free energy functional into a larger space, so that it bears all the symmetries explicitly and, of course, generates all the thermodynamics as well.

2. HARD-ROD FLUID ON A LATTICE

We begin by looking at a lattice gas with core length m, i.e., a particle excludes m contiguous sites on each side from occupation by other particles. We denote by $n(v_{x+1},..., v_{x+s})$ the s-tuple distribution for the specified configuration at the sites $x+1,..., x+s$: $v_x = x$ if x is occupied; $v_x = \bar{x}$ if it is empty. We also define

$$n^-(v_{x+1},..., v_{x+s}) \equiv n(..., \overline{x-1}, \bar{x}, v_{x+1},..., v_{x+s}) \tag{1}$$

$$n^+(v_{x+1},..., v_{x+s}) \equiv n(v_{x+1},..., v_{x+s}, \overline{x+s+1}, \overline{x+s+2},...) \tag{2}$$

Due to the hard-core nature, we obviously have the following probability relations:

$$\begin{aligned} n(x) &= P(x \mid \overline{x-m},..., \overline{x-1})\, n(\overline{x-m},..., \overline{x-1}) \\ &= \frac{n^-(x)}{n^-(x)+n^-(\bar{x})}\, n(\overline{x-m},..., \overline{x-1}) \end{aligned} \tag{3}$$

$$n(x) = P(x \mid \overline{x+1},..., \overline{x+m})\, n(\overline{x+1},..., \overline{x+m}) \tag{4}$$

$$= \frac{n^+(x)}{n^+(x)+n^+(\bar{x})}\, n(\overline{x-m},..., \overline{x+1}) \tag{5}$$

where P is the conditional probability. These relations result in a pair of important equations which will be called the "characteristic equations" (CE),

$$\frac{n^-(\bar{x})}{n^-(x)} = \frac{n(\overline{x-m},..., \overline{x-1}, \bar{x})}{n(x)} \tag{6}$$

$$\frac{n^+(\bar{x})}{n^+(x)} = \frac{n(\bar{x}, \overline{x+1},..., \overline{x+m})}{n(x)} \tag{7}$$

Let u_x be an arbitrary external potential field, so that the probability of putting a particle at x is proportional to

$$w_x \equiv e^{\mu(x)} \equiv e^{\mu - u_x}$$

where μ is the chemical potential and $\beta = 1/kT$ has been set to unity for convenience.

To find the (inverse) profile, namely to express the external field in terms of the particle densities, we form a local product

$$\frac{n(\overline{x-m+1},..., \bar{x})}{w_x n(x)} \frac{n(\overline{x-m+2},..., \overline{x+1})}{w_x n(x)} \cdots \frac{n(\bar{x},..., \overline{x+m-1})}{w_x n(x)} \tag{8}$$

By the definitions, this may also be written as

$$\frac{n^-(\bar{x})\, n^+(\overline{x-m+1})}{n^-(x)\, n^+(x)} \frac{n^-(\overline{x+1})\, n^+(\overline{x-m+2})}{n^-(x)\, n^+(x)} \cdots \frac{n^-(\overline{x+m-1})\, n^+(\bar{x})}{n^-(x)\, n^+(x)} \tag{9}$$

or, regrouping terms,

$$\frac{n^-(\bar{x})}{n^-(x)} \frac{n^+(\overline{x-m+1})\, n^-(\overline{x+1})}{n^+(x)\, n^-(x)} \cdots \frac{n^+(\overline{x-1})\, n^-(\overline{x+m-1})}{n^+(x)\, n^-(x)} \frac{n^+(\bar{x})}{n^+(x)} \tag{10}$$

Replacing the end factors by the "characteristic equations" (6) and (7) and transforming each factor in the middle by its definition, (10) yields

$$\frac{n(\overline{x-m},..., \bar{x})}{n(x)} \frac{n(\overline{x-m+1},..., \overline{x+1})}{w_x n(x)} \cdots \cdots \frac{n(\overline{x-1},..., \overline{x+m-1})}{w_x n(x)} \frac{n(\bar{x},..., \overline{x+m})}{n(x)} \tag{11}$$

Comparing this with (8), we conclude that

$$\begin{aligned} \frac{w_x}{n(x)} &= \frac{n(\overline{x-m+1},..., \bar{x})\, n(\overline{x-m+2},..., \overline{x+1}) \cdots n(\bar{x},..., \overline{x+m-1})}{n(\overline{x-m},..., \bar{x})\, n(\overline{x-m+1},..., \overline{x+1}) \cdots n(\bar{x},..., \overline{x+m})} \\ &= \frac{\prod_{k=1}^{m} [1 - \sum_{j=1}^{m+1} n(x+k-j)]}{\prod_{k=1}^{m+1} [1 - \sum_{j=1}^{m} n(x+k-j)]} \end{aligned} \tag{12}$$

which is the exact (inverse) profile equation for the nonuniform hard-rod fluid on a lattice.

3. CONTINUUM FLUID AND LOCAL PRESSURE FIELDS

One could go ahead and take the continuum limit of (12), but it is more instructive to proceed differently. All the essential features of the system are captured in CE, i.e., (6) and (7). We would like to find the local pressure fields by varying the core size while keeping the particle density fixed. For this purpose, let us rewrite (6) as

$$\begin{aligned}
&\ln n(\overline{x-m},..., \bar{x}) \\
&\quad = -\ln \frac{n^-(x; m)}{n^-(\bar{x}; m)} + \ln n(x) \\
&\quad = -\left(\ln \frac{n^-(x; m)}{n^-(\bar{x})} - \ln \frac{n^-(x; m-1)}{n^-(\bar{x}; m-1)} \right) \\
&\qquad - \cdots - \left(\ln \frac{n^-(x; 1)}{n^-(\bar{x})} - \ln \frac{n^-(x; 0)}{n^-(\bar{x}; 0)} \right) + \ln[1 - n(x)] \\
&\quad \equiv -[p_x^-(m) - p_x^-(m-1)] - \cdots - [p_x^-(1) - p_x^-(0)] + \ln[1 - n(x)]
\end{aligned}$$

where we have indicated the core dependences, and $p_x^-(m)$ may be regarded as the effective left pressure field (i.e., to the left of x) in a fluid of core size m. In the continuum limit, one has to rescale n to be unity at close packing, and the above equation becomes

$$-\int_0^a dt\, p_x^-(t) = \ln \left[1 - \int_{x-a}^{x} dy\, n(y) \right] \tag{13}$$

or

$$p_x^-(a) = \frac{n(x-a)}{1 - \int_{x-a}^{x} dy\, n(y)} \tag{14}$$

Notice that we have used the same notations for the continuum variables. Similarly, if we start with (7), we end up with

$$-\int_0^a dt\, p_x^+(t) = \ln \left[1 - \int_{x}^{x+a} dy\, n(y) \right] \tag{15}$$

or

$$p_x^+(a) = \frac{n(x+a)}{1 - \int_{x}^{x+a} dy\, n(y)} \tag{16}$$

where $p_x^+(a)$ is the effective right pressure (i.e., to the right of x) in the fluid. Therefore, the corresponding truncated partition functions are simply given by

$$\Xi_x^-(a) = \exp \int_{-\infty}^{x} dy\, p_y^-(a) \tag{17}$$

$$\Xi_x^+(a) = \exp \int_{x}^{\infty} dy\, p_y^+(a) \tag{18}$$

With the symmetric pressure

$$p_x(a) = \tfrac{1}{2}[p_{x+a/2}^-(a) + p_{x-a/2}^+(a)]$$

and the total grand partition function

$$\Xi(a) = \exp \int_{-\infty}^{\infty} dx\, p_x(a) = \Xi_\infty^-(a) = \Xi_{-\infty}^+(a)$$

the (inverse) profile is, of course, given by

$$w_x = \frac{n(x)\,\Xi}{\Xi_x^- \Xi_x^+} \tag{19}$$

4. REVERSING THE LOGIC

Now we would like to reverse the logic: varying the core from the very beginning of the game. Hence we extend the idea of RFL[6] to the nonuniform case. The physics is the same: the probability of creating an empty core of size a at x is equal to the Boltzmann factor corresponding to the total reversible work done. We can do this in three natural ways:

1. Symmetrically:

$$1 - \int_{x-a/2}^{x+a/2} dy\, n(y) = \exp - \int_0^a dt\, p_x(t) \equiv \exp f_x(a) \equiv Z_x^0(a) \tag{20}$$

2. To the left:

$$1 - \int_{x-a}^{x} dy\, n(y) = \exp - \int_0^a dt\, p_x^-(t) \equiv \exp f_x(a) \equiv Z_x^-(a) \tag{21}$$

3. To the right:

$$1 - \int_{x}^{x+a} dy\, n(y) = \exp - \int_0^a dt\, p_x^+(t) \equiv \exp f_x^+(a) \equiv Z_x^+(a) \tag{22}$$

Of these, only one is independent; Z^- and Z^+ are related by the symmetry transformation $a \to -a$, $n \to -n$. Hence locally, a Z-function will determine everything. We also call these CE—"characteristic equations." They play a rather important role, as they satisfy linear hyperbolic equations. $Z^{\pm}$ satisfy the first-order inhomogeneous equations

$$(\partial_a \pm \partial_x)\, Z_x^{\mp}(a) = \pm n(x) \tag{23}$$

with the same initial condition $Z_x^{\pm}(0) = 1$; $Z_x^0(a)$ satisfies the wave equation (think of a as the time)

$$(\partial_{aa}^2 - v^2 \partial_{xx}^2)\, Z_x^0(a) = 0$$

with the inital conditions $Z_x^0(0) = 1$, $\partial_a Z_x^0(0) = -n(x)$, and the speed $v = 2$. The physical meanings of these equations and initial conditions are clear: they form the differential CE and the solutions are certainly unique.

Once we know a Z-function, Z^- say, we can follow the same procedure as in the last section to get the (inverse) profile,

$$\begin{aligned} \ln n(x) - \mu(x) &= \int_{-\infty}^{x} dz\, [p_z^-(a) - p_z^+(a)] \\ &= \ln Z_x^-(a) - \int_x^{x+a} dz\, \frac{n(z)}{Z_z^-(a)} \end{aligned} \tag{24}$$

and get all the direct correlation functions by differentiation[7]

$$c_s(x_1, \ldots, x_s) = \frac{\delta^{s-1}[-\mu(x_1) + \ln n(x_1)]}{\delta n(x_2) \cdots \delta n(x_s)} \tag{25}$$

In particular, if $x \leqslant y \leqslant x + a$,

$$c_2(x, y) = \frac{-1}{Z_y^-(a)} - \int_y^{x+a} dz\, \frac{n(z)}{[Z_z^-(a)]^2} \tag{26}$$

5. A VARIATIONAL PROBLEM

For the hard-rod fluid, it turns out that c_2 can be calculated directly as a Riemann–Hilbert problem by using the well-known Wiener–Hopf factorization technique.[2] We would like to connect this to a variational

[2] This was done by Baxter[8] for the uniform system in three dimensions under the PY condition, which is exact in one dimension (M. Wertheim and E. Thiele had done this earlier using different techniques). Extension to the 1D nonuniform case was done in ref. 2. For the Wiener–Hopf techniques, one may refer to, e.g. Noble.[9]

problem that Dyson had considered when studying the Gelfand–Levitan construction in the inverse scattering theory of quantum mechanics.[10]

Recall the modified pair Ursell function:

$$\begin{aligned} S(x, y) &= \langle [\rho(x) - n(x)][\rho(y) - n(y)] \rangle \\ &= n(x)\,\delta(x-y) + n_2(x, y) - n(x)\,n(y) \\ &\equiv n(x)\,\delta(x-y) + H(x-y) \end{aligned}$$

with $\rho(x)$ being the microscopic density $\sum_i \delta(x - x_i)$. We multiply the above equation by $n^{-1/2}(x)$ from the left and $n^{-1/2}(y)$ from the right, and rewrite it in operator form

$$\hat{S} = 1 + \hat{H}$$

with the obvious definitions $\hat{S} = n^{-1/2} S n^{-1/2}$ and $\hat{H} = n^{-1/2} H n^{-1/2}$. Clearly, $\hat{S}$ is positive definite and has an inverse, which we denote by

$$\hat{C} \equiv 1 - \hat{c}_2$$

so that

$$\hat{H} = \hat{c}_2(1 - \hat{c}_2), \qquad \hat{c}_2 = \hat{H}(1 + \hat{H}) \tag{27}$$

Here $c_2 = n^{-1/2} \hat{c}_2 n^{-1/2}$ is just the Ornstein–Zernike pair direct correlation function (25). Let P_t be the diagonal kernel

$$P_t(x, y) = \delta(x - y) \qquad \text{for} \quad x, y > t; \qquad = 0 \quad \text{otherwise}$$

We consider the quantity

$$W_t(K) = \mathrm{Tr}[P_t(KK^\dagger + (1 + K)\,\hat{H}(1 + K^\dagger))] \tag{28}$$

which is a functional bilinear in the kernel K and its adjoint $K^\dagger$. A little algebra shows that

$$W_t(K) = \mathrm{Tr}[P_t(\hat{c}_2 + (K + \hat{c}_2)\,\hat{S}(K^\dagger + \hat{c}_2))] \geqslant \mathrm{Tr}[P_t \hat{c}_2] \tag{29}$$

so that W is bounded below for all K. Let K now belong to the class of causal kernels, that is,

$$K(x, y) = 0 \qquad \text{for} \quad x > y$$

Within this class, $W_t(K)$ is still bounded below and attains its minimum value

$$M_t = W_t(\hat{A})$$

for a particular causal kernel $\hat{A}$ which is independent of t. The variation of (28) gives rise to the Marchenko equation[11]

$$[\hat{A}+\hat{H}+\hat{A}\hat{H}](x, y)=0 \qquad \text{for} \quad y>x \tag{30}$$

which is a linear integral equation of Fredholm type which determines the kernel $\hat{A}$ uniquely. This equation is equivalent to

$$\hat{A}+\hat{H}+\hat{A}\hat{H}=\hat{B}^{\dagger} \tag{31}$$

for another causal kernel $\hat{B}$. From this, it follows that

$$(1+\hat{B}^{\dagger})(1+\hat{A}^{\dagger})=(1+\hat{A})\,\hat{S}(1+\hat{A}^{\dagger})$$

But the right-hand side is self-adjoint, while the left is the unit operator plus an anticausal kernel. Therefore both sides must be equal to unity, and we have

$$(1+\hat{A})(1+\hat{B})=1$$

Combining this with (27) and (31), we find

$$\hat{S}=1+\hat{H}=(1+\hat{B})(1+\hat{B}^{\dagger}) \tag{32}$$

$$\hat{C}=1-\hat{c}_2=(1+\hat{A}^{\dagger})(1+\hat{A}) \tag{33}$$

The last equation is a nonlinear integral equation for $\hat{A}$, sometimes called the nonlinear Gelfand–Levitan equation.[12] Using these equations together with (31) and rewriting (28) in the form

$$W_t(K)=\mathrm{Tr}[P_t(\hat{B}+\hat{B}^{\dagger}+(K-\hat{A})\,\hat{S}(K^{\dagger}-\hat{A}^{\dagger}))] \tag{34}$$

valid for any causal kernel K, we see explicitly that the minimum value

$$M_t=\mathrm{Tr}[P_t(\hat{B}+\hat{B}^{\dagger})]$$

of $W_t(K)$ is attained at $K=\hat{A}$ for every value of t. Dyson then went forward to show that if $\hat{H}$ represents the spectral function, then the corresponding quantum mechanical potential in the Schrödinger equation is given by

$$V(x)=-2\frac{d^2}{dx^2}M_x=-2\frac{d^2}{dx^2}\ln \mathrm{Det}\,\hat{S}\Big|_x^{\infty}$$

For our special system—a classical hard-rod fluid—$\hat{C}$ is short-ranged; in particular, $\hat{A}$ has only a range of a. More importantly, $n_2(x, y)=0$ for

$|x-y| \leqslant a$, so that the Marchenko equation (30) becomes a simple linear equation for $\hat{A}(x, y)$ in its range: $x \leqslant y \leqslant x+a$,

$$\hat{A}(x, y) - n^{1/2}(x)\, n^{1/2}(y) - \int_x^{x+a} dz\, \hat{A}(x, z)\, n^{1/2}(z)\, n^{1/2}(y) = 0 \tag{35}$$

and the solution is

$$\begin{aligned} \hat{A}(x, y) &= n^{1/2}(x) \frac{\varepsilon(y-x)\, \varepsilon(x+a-y)}{Z_x^+(a)} n^{1/2}(y) \\ &= -n^{1/2}(x) \frac{\delta f_x^+(a)}{\delta n(y)} n^{1/2}(y) \end{aligned} \tag{36}$$

where $f_x^+(a) = \ln Z_x^+(a)$ is defined in (22). We see again the presence of the "characteristic" Z-function. According to (33),

$$c_2 = n^{-1/2} \hat{c}_2 n^{-1/2} = -n^{-1/2} [\hat{A}^\dagger + \hat{A} + \hat{A}^\dagger \hat{A}]\, n^{-1/2} \tag{37}$$

which may be checked as agreeing with (26).

We now make some comments. In order: (a) The factorizations (32), (33) are very general, regardless of the range of the operators; they depend only upon the topological nature of $\mathbf{R}$, i.e., space can be disconnected by a point. (b) On the other hand, it is often the case that one operator has much shorter range than its inverse. For physical systems with short-range interactions, it is always $\hat{C}$ that has a shorter range, which is usually comparable to that of the interactions except near some critical points. (c) It is the peculiarity of a hard-rod system that $c_2(x, y) = 0$ for $|x-y| > a$ (this is only approximately true for hard disks or spheres). This together with $n_2(x, y) = 0$ for $|x-y| \leqslant a$ allows a successful Wiener–Hopf treatment.

Why should there be such a variational principle in the first place? To motivate his formulation of the inverse scattering theory, Dyson had to resort to an artificial analogy with optics,[13] which in turn is a special case of the general problem of optimization of a linear control system (see, e.g., Kailath[14]). This reminds us of the Galerkin method used in the hole theory[15,16] of fluids. If we define

$$\rho_h(r) = \exp\left[\mu(r) - \sum_i \phi(r, r_i)\right]$$

where $\phi(r, r')$ is the pair interaction potential, then it is remarkable that

$$\langle \rho_h(r) \rangle = \langle \rho(r) \rangle = n(r)$$

It is then natural to assume that the fluctuations $\delta\rho_h(r) = \rho_h(r) - n(r)$ and $\delta\rho(r) - n(r)$ are approximately linearly related, so that the dimensionless quantity

$$D(r) = \frac{\delta\rho_h(r)}{n(r)} - \int dr'\, G(r, r')\, \frac{\delta\rho(r')}{n(r')}$$

would be "small" for suitably chosen G. It can be shown that the correlation function (kernel of integral operator)

$$\Delta(r, r') = \langle D(r)\, D(r') \rangle \geqslant 0$$

is positive semidefinite and is equal to (in operator form)

$$\Delta = y - g + c_2 + (G - c_2 n)(n^{-1} H n^{-1} + n^{-1})(G - c_2 n)^\dagger \tag{38}$$

where $y(r, r') = g(r, r')\, e^{\phi(r,r')}$ and $g = 1 + n^{-1/2} H n^{-1/2}$. We can minimize Δ by choosing

$$G = c_2 n$$

so that

$$\Delta_{\min} = y - g + c_2 \geqslant 0 \tag{39}$$

$$D = n^{-1}\, \delta\rho_h - c_2\, \delta\rho \tag{40}$$

The PY approximation is precisely the statement that

$$\Delta_{\min} = y - g + c_2 = 0 \tag{41}$$

For our hard-rod system, this approximation gives the exact c_2! Comparing with (29), we see essentially that

$$K = -n^{1/2} G n^{-1/2} \qquad \text{and} \qquad W_t = \operatorname{Tr} P_t[D - (y - g)]$$

Therefore, by using the particle–hole symmetry of fluids, (39) gives a much sharper bound.

6. SYMMETRIES AND A LIFTED GLOBAL FUNCTIONAL

The fact that the symmetries (a) particle–hole, (b) hard rod [this refers to the symmetry that the system can be described by different Z-functions; it is well known that the expressions for $\mu(x)$ and $c_2(x, y)$ take the guise of many different but equivalent forms] and (c) one dimension make the hard-rod statistical mechanics exactly solvable may prompt us to ask deeper questions. What really are these symmetries? After all, we know very well why there is a minimization principle, because there exists a convex free energy functional. Can we push the idea of treating the core size as an extra independent degree of freedom and thus lift up the whole global functional? If we can, all the symmetries that we mentioned above would manifest themselves explicitly. The answer is affirmative.

Let us consider all hard-rod systems with core size from 0 to $b \geqslant a$. Every member of this "super" ensemble may be generated by two independent procedures: (1) choosing a location $-\infty < x < \infty$ for a rod; (2) increasing reversibly the core from 0 to b. Since there is no integral energy involved, the free energy in a given density is essentially the entropy. We define a "super" free energy functional by

$$F_{\mathrm{sup}}[n; b] = \int dx \, \{b[n(x) \ln n(x) - 1] + Z_x(b)[\ln Z_x(b) - 1]\} \quad (42)$$

Here Z could be any of $Z^{\pm}$ and Z^0, remembering that the "characteristic" Z-function is the (normalized) probability density of creating a hole. Then, the ordinary free energy density functional for a hard-rod system of core size a can be obtained by differentiating the "super" F_{sup}:

$$F[n] = \left.\frac{\partial}{\partial b}\right|_{b=a} F_{\mathrm{sup}}[n; b]$$

For instance, if we choose Z^-,

$$F = \int dx \, \{n(x)[\ln n(x) - 1] - p_x^-(a) \ln Z_x^-(a)\}$$

since $Z_x^-(0) = 1$, F would reduce to the ideal-gas free energy in the limit $a \to 0$, as it should. To calculate the (inverse) profile, we start with

$$\mu(x) = \frac{\delta F}{\delta n(x)} = \ln n(x) + \frac{\delta}{\delta n(x)} \int dy \, \frac{\partial Z_y^-(a)}{\partial a} \ln Z_y^-(a)$$

using the differential equation (23) satisfied by Z^-,

$$\mu(x) = \ln n(x) + \frac{\delta}{\delta n(x)} \int dy \left[n(y) - \frac{\partial Z_y^-(a)}{\partial y} \right] \ln Z_y^-(a)$$

The last term involving a total integration can be thrown away; we finally obtain

$$\mu(x) = \ln n(x) + \ln Z_x^- - \int_x^{x+a} dy \, \frac{n(y)}{Z_y^-(a)}$$

which is just (24). One can calculate all the direct correlation functions by taking further functional derivatives of F with respect to n's.

Indeed, now the symmetry is more evident in F_{sup}, (42). In particular, the choice of a different Z-function corresponds to a different shift of x, while the integration makes F_{sup} (and hence F itself) invariant under such a shift.

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