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Entropy of a non-uniform one-dimensional fluid†

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Abstract. A one-dimensional particle system with arbitrary nearest-neighbour interaction and arbitrary external field is investigated. The system is considered as an inverse problem, that of determining the internal and external interactions needed to produce given singlet and nearest-neighbour pair densities. The profile equations, the entropy functional which generates them, and the redefined direct correlation function are found exactly. Equivalent expressions are derived in which the full pair distribution and potential-range truncation are the controlling functions.

1. Introduction

Much of the qualitative information we possess on the properties of many-body systems comes from exactly solvable models. Exact solvability in this context of course means reduction to a space whose dimensionality does not change with the number of particles. Even at this level, however, there is a large distinction between solvability in principle and the exhibiting of explicit solutions which aid and may even direct the construction of the intuitive conceptual framework which we equate with understanding. Equilibrium classical statistical mechanics has a particularly simple mathematical formulation, and so one might anticipate that relevant models could be constructed without difficulty. This is not the case, and for pair-interacting particle systems controlled by external fields, only a few one-dimensional fluids and a very special two-dimensional fluid fall into this category [1]. The purpose of this paper is to show that a modest expansion of the meaning of solvability leads to the complete solution of a more substantial class of one-dimensional fluids, and to a simplification of associated structural parameters.

The system we have in mind is that of particles on a line in equilibrium at reciprocal temperature β. They interact via a pair potential $\phi(x, x')$ and are subject to an external potential $u(x)$ which serves for containment as well. In a grand ensemble at chemical potential μ, the system properties are completely determined by the grand potential

$$\Omega[\mu - u, \phi]. \tag{1.1}$$

In particular, the mean particle density is given by

$$n(x) = -\delta\Omega/\delta(\mu - u(x)) \tag{1.2}$$

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and the pair density by

$$n_2(x, x') = 2\delta\Omega/\delta\phi(x, x'). \tag{1.3}$$

Before proceeding further, we will, however, confine our consideration to a simple but still significant subclass of systems, that in which the pair potential $\phi(x, x')$ is limited to nearest-neighbour particles. (This makes physical sense if non-adjacent particles cannot interact: $\phi(x - x') = \infty$ for $|x - x'| \leq a$, but $\phi(x, x') = 0$ for $|x - x'| \geq 2a$—but we will not yet impose such a detailed condition.) If ϕ is so restricted, we will also declare it to be defined only for $x' \geq x$; thus (1.3) is replaced by

$$\bar{n}_2(x, x') = \delta\Omega/\delta\phi(x, x') \tag{1.4}$$

where $\bar{n}_2$ is the nearest-neighbour pair distribution, also restricted to $x' \geq x$.

It is now our intention to allow both u and ϕ to be chosen at will —within the nearest-neighbour context—resulting in equally arbitrary profile $n(x)$ and pair profile $\bar{n}_2(x, x')$. We will do this, however, by expressing all quantities in terms of n and $\bar{n}_2$, from which u and ϕ can be derived. It is this change of viewpoint [2] that leads to the possibility of effective solvability. To convert our description from u and ϕ as basic functions to n and $\bar{n}_2$, we perform a Legendre transformation:

$$\begin{aligned} A = \int (\mu - u(x)) \frac{\delta\Omega}{\delta\mu - u(x)} \, \mathrm{d}x + \int\int \phi(x, x') \frac{\delta\Omega}{\delta\phi(x, x')} \, \mathrm{d}x \, \mathrm{d}x' - \Omega \\ = -\mu \int n(x) \, \mathrm{d}x + \int u(x) n(x) \, \mathrm{d}x + \int\int \phi(x, x') \bar{n}_2(x, x') \, \mathrm{d}x \, \mathrm{d}x' - \Omega \end{aligned} \tag{1.5}$$

which we recognise as the thermodynamic function $-G + U + PV = TS$ and shall so denote it. Regarding $TS[n, \bar{n}_2]$ as a functional of n and $\bar{n}_2$, we then find from (1.2) and (1.4) the associated conjugate relations

$$u(x) - \mu = \frac{\delta TS}{\delta n(x)} \qquad \phi(x, x') = \frac{\delta TS}{\delta \bar{n}_2(x, x')}. \tag{1.6}$$

Our task is to construct the entropy functional $TS[n, \bar{n}_2]$, equations (1.6) constituting a complete solution in inverse form of the profile problem at the one- and (nearest-neighbour) two-body levels, with thermodynamics being picked up at leisure.

2. Basic solution

Let us start with an N-particle canonical ensemble. The (coordinate part of the) partition function is thus given, in obvious notation, by

$$\begin{aligned} Q_N = \int_{1 \leq \ldots \leq N} \cdots \int \exp(-\beta u(1)) \exp(-\beta\phi(1, 2)) \exp(-\beta u(2)) \ldots \exp(-\beta\phi(N-1, N)) \\ \times \exp(-\beta u(N)) \, \mathrm{d}1 \cdots \mathrm{d}N \end{aligned} \tag{2.1}$$

where ordering the particles has removed the standard $1/N!$ indistinguishability factor. An even more concise notation is useful. We introduce the matrix, diagonal matrix and special vector:

$$\begin{aligned}\langle 1|w|2\rangle &= \exp(-\beta\phi(1,2))\epsilon(x_2-x_1)\\ \langle 1|e|2\rangle &= e(1)\delta(x_2-x_1)\\ \langle J|1\rangle &= 1\end{aligned} \tag{2.2}$$

where $e(1)=\exp(-\beta u(1))$, (2.1) thereby appearing as

$$Q_N = \langle J|(ew)^{N-1}e|J\rangle. \tag{2.3}$$

Similarly, the one-body density $n(1)$ in which one of the particles is fixed at x_1, is given by

$$n_N(1)Q_N = \sum_{i=1}^{N}\langle J(ew)^{i-1}|1\rangle\langle 1|(ew)^{N-i}e|J\rangle \tag{2.4}$$

and the nearest-neighbour pair distribution (with $x_1 \leq x_2$ automatically enforced) by

$$\overline{n}_{2N}(1,2)Q_N = \sum_{i=1}^{N-1}\langle J|(ew)^{i-1}|1\rangle\langle 1|ew|2\rangle\langle 2|(ew)^{N-2-i}|J\rangle. \tag{2.5}$$

We now proceed to the grand ensemble, in which momentum integrations are as usual incorporated into the definition of the chemical potential. To start with,

$$\Xi = \sum_N \exp(N\beta\mu)Q_N = 1 + \langle J|(I-zw)^{-1}|J\rangle \tag{2.6}$$

where $\langle 1|z|2\rangle = \exp[\beta(\mu-u(1))]\delta(1,2)$. Continuing,

$$n(1)\Xi = \sum_N \exp(N\beta\mu)n_N(1) = \langle J|(I-zw)^{-1}|1\rangle z(1)\langle 1|(I-wz)^{-1}|J\rangle \tag{2.7}$$

and in the same fashion

$$\overline{n}_2(1,2)\Xi = \langle J|(I-zw)^{-1}|1\rangle z(1)\langle 1|w|2\rangle z(2)\langle 2|(I-wz)^{-1}|J\rangle. \tag{2.8}$$

To express all relevant quantities in terms of n and $\overline{n}_2$, we regard $\overline{n}_2(1,2)$ as a matrix $\langle 1|\overline{n}_2|2\rangle$ and n as a diagonal matrix. We first observe, from (2.7) and (2.8), that

$$\langle 1|\overline{n}_2 n^{-1}|2\rangle = \langle (I-zw)^{-1}|1\rangle z(1)\langle 1|w|2\rangle / \langle (I-zw)^{-1}|2\rangle \tag{2.9}$$

where the omission of a left or right vector in a matrix element is hereafter interpreted as the presence of the standard vector $\boldsymbol{J}$. It follows that

$$\langle 1|I-\overline{n}_2 n^{-1}|2\rangle = \langle (I-zw)^{-1}|1\rangle\langle 1|I-zw|2\rangle / \langle (I-zw)^{-1}|2\rangle \tag{2.10}$$

as well as

$$\langle 1|(I-\overline{n}_2 n^{-1})n\rangle = \langle (I-zw)^{-1}|1\rangle\langle 1|I-zw|2\rangle z(2)\langle 2|(I-wz)^{-1}\rangle/\Xi. \tag{2.11}$$

Integrating over 2, then

$$\langle 1|(I-\bar{n}_2 n^{-1})n\rangle = \langle (I-zw)^{-1}|1\rangle z(1)/\Xi \tag{2.12}$$

and over 1,

$$\langle (I-\bar{n}_2 n^{-1})n\rangle = \langle (I-zw)^{-1}z\rangle/\Xi = (\Xi-1)/\Xi. \tag{2.13}$$

We then have the first of the thermodynamic quantities

$$\Xi = 1/[1-\langle (I-\bar{n}_2 n^{-1})n\rangle]. \tag{2.14}$$

As for the profile equations, (2.10) tells us that

$$\langle (I-\bar{n}_2 n^{-1})|2\rangle = 1/\langle (I-zw)^{-1}|2\rangle \tag{2.15}$$

and so from (2.12) and (2.14),

$$z(1) = \frac{\langle I-\bar{n}_2 n^{-1}|1\rangle n(1)\langle 1|I-n^{-1}\bar{n}_2\rangle}{1-\langle (I-\bar{n}_2 n^{-1})n\rangle}. \tag{2.16}$$

From the relation

$$\langle 1|I-n^{-1}\bar{n}_2\rangle = 1/\langle 1|(I-wz)^{-1}\rangle \tag{2.17}$$

derived as was (2.15), equation (2.8) is then readily converted, via (2.14)–(2.16) to read

$$\langle 1|w|2\rangle = \frac{\langle 1|n^{-1}\bar{n}_2 n^{-1}|2\rangle[1-\langle (I-\bar{n}_2 n^{-1})n\rangle]}{\langle 1|I-n^{-1}\bar{n}_2\rangle\langle I-\bar{n}_2 n^{-1}|2\rangle}. \tag{2.18}$$

Taking logarithms, (2.16) and (2.18) yield the profile equations

$$\beta(u(1)-\mu) = \ln[1-\langle (I-\bar{n}_2 n^{-1})n\rangle] - \ln n(1) - \ln\langle I-\bar{n}_2 n^{-1}|1\rangle - \ln\langle 1|I-n^{-1}\bar{n}_2\rangle \tag{2.19}$$

and

$$\beta\phi(1,2) = \ln\langle 1|I-n^{-1}\bar{n}_2\rangle + \ln\langle I-\bar{n}_2 n^{-1}|2\rangle - \ln\langle 1|n^{-1}\bar{n}_2|2\rangle - \ln[1-\langle (I-\bar{n}_2 n^{-1})\rangle]. \tag{2.20}$$

Finally, the desired generating function $TS(n,\bar{n}_2)$ is obtained by direct substitution of (2.14), (2.19) and (2.20) into (1.5), using of course the identification $\Omega = -\beta^{-1}\ln\Xi$. This results in

$$\begin{aligned} -S/\kappa = {} & \int\!\!\int \bar{n}_2(1,2)\ln\bar{n}_2(1,2)\,\mathrm{d}1\,\mathrm{d}2 - \int n(1)\ln n(1)\,\mathrm{d}1 \\ & + \int\left(n(1)-\int\bar{n}_2(1,2)\,\mathrm{d}2\right)\ln\left(n(1)-\int\bar{n}_2(1,2)\,\mathrm{d}2\right)\mathrm{d}1 \\ & + \int\left(n(1)-\int\bar{n}_2(2,1)\,\mathrm{d}2\right)\ln\left(n(1)-\int\bar{n}_2(2,1)\,\mathrm{d}2\right)\mathrm{d}1 \\ & + \left(1-\int n(1)\,\mathrm{d}1 + \int\!\!\int\bar{n}_2(1,2)\,\mathrm{d}1\,\mathrm{d}2\right) \\ & \times\ln\left(1-\int n(1)\,\mathrm{d}1+\int\!\!\int\bar{n}_2(1,2)\,\mathrm{d}1\,\mathrm{d}2\right). \end{aligned} \tag{2.21}$$

As a check, we may apply the relations (1.6), which give (2.19) and (2.20) in the form

$$\beta(u(1)-\mu) = \ln n(1) - \ln\left(n(1) - \int \bar{n}_2(1,3)\,\mathrm{d}3\right) - \ln\left(n(1) - \int \bar{n}_2(3,1)\,\mathrm{d}3\right) + \ln\left(1 - \int n(3)\,\mathrm{d}3 + \int\int \bar{n}_2(3,4)\,\mathrm{d}3\,\mathrm{d}4\right) \tag{2.22a}$$

$$\beta\phi(1,2) = -\ln \bar{n}_2(1,2) + \ln\left(n(1) - \int \bar{n}_2(1,3)\,\mathrm{d}3\right) + \ln\left(n(2) - \int \bar{n}_2(3,2)\,\mathrm{d}3\right) - \ln\left(1 - \int n(3)\,\mathrm{d}3 + \int\int \bar{n}_2(3,4)\,\mathrm{d}3\,\mathrm{d}4\right). \tag{2.22b}$$

3. Relationship to previous work

One-dimensional fluids with nearest-neighbour interaction and arbitrary external field have been considered on previous occasions, and a meagre number of these systems solved exactly [3,4]. We are not going to solve any previously unsolved instances in the previous phraseology, but it is appropriate—and easy—to relate the present viewpoint to prior formulations. For this purpose, it is necessary to eliminate the dependence upon the pair distribution $\bar{n}_2$. To do so, we rewrite the second of (2.22) as

$$\bar{n}_2(1,2) = w(1,2)\left(n(1) - \int \bar{n}_2(1,3)\,\mathrm{d}3\right)\left(n(2) - \int \bar{n}_2(3,2)\,\mathrm{d}3\right)\Xi. \tag{3.1}$$

Then define

$$Z(1) = \frac{n(1)}{n(1) - \int \bar{n}_2(1,3)\,\mathrm{d}3} \tag{3.2}$$

$$\hat{Z}(2) = \frac{n(2)}{n(2) - \int \bar{n}_2(3,2)\,\mathrm{d}3} \tag{3.3}$$

so that

$$\bar{n}_2(1,2) = w(1,2)\frac{n(1)n(2)}{Z(1)\hat{Z}(2)}\Xi. \tag{3.4}$$

Now integrating (3.4) over 2, we have

$$n(1) - \frac{n(1)}{Z(1)} = \frac{n(1)}{Z(1)}\Xi \int \frac{w(1,3)n(3)}{\hat{Z}(3)}\,\mathrm{d}3$$

or

$$Z(1) = 1 + \Xi \int \frac{w(1,3)n(3)}{\hat{Z}(3)}\,\mathrm{d}3 \tag{3.5}$$

whereas integrating (3.4) over 1 similarly yields

$$\hat{Z}(2) = 1 + \Xi \int \frac{w(3,2)n(3)}{Z(3)}\,\mathrm{d}3. \tag{3.6}$$

These, coupled with the relation

$$n(1) = z(1)Z(1)\hat{Z}(1)/\Xi \tag{3.7}$$

which comes at once from (2.22), and the identification

$$\Xi = \left(1 - \int \frac{n(1)}{Z(1)}\,\mathrm{d}1\right)^{-1} = \left(1 - \int \frac{n(1)}{\hat{Z}(1)}\,\mathrm{d}1\right)^{-1} \tag{3.8}$$

are recognised as the profile equations previously obtained [4], with $Z(1)$ and $\hat{Z}(1)$ representing truncated partition functions.

The direct correlation function c_2 is a quantity that has previously been investigated in some detail. The often more convenient complete direct correlation function or linear response

$$\frac{\delta(1,2)}{n(1)} - c_2(1,2) = C(1,2) = \left.\frac{\delta\beta(\mu - u(1))}{\delta n(2)}\right|_{\phi} \tag{3.9}$$

for the present systems is not especially simple or transparent, and will be referred to in §4. However, it is important to observe that if the response is taken, not at fixed ϕ, but at fixed $\bar{n}_2$, then we have instantly from (2.22)

$$\begin{aligned} C'(1,2) &= \left.\frac{\delta\beta(\mu - u(1))}{\delta n(2)}\right|_{\bar{n}_2} \\ &= \left(\frac{1}{n(1) - \int \bar{n}_2(1,3)\,\mathrm{d}3} + \frac{1}{n(1) - \int \bar{n}_2(3,1)\,\mathrm{d}3} - \frac{1}{n(1)}\right)\delta(1,2) \\ &\quad + \frac{1}{1 - \int n(3)\,\mathrm{d}3 + \int\int \bar{n}_2(2,3)\,\mathrm{d}2\,\mathrm{d}3} \end{aligned} \tag{3.10}$$

the sum of a zero-range part and a constant. The net effect is that in our expanded format, the direct correlation regains the simplicity—and short-range non-trivial part—that held previously only for hard-rod interactions.

4. Extension to full pair distribution

Since $\bar{n}_2$ is not itself an observable quantity, it makes more sense to convert our formulation to one in which the full pair distribution $n_2(1,2)$ appears, if feasible. It is simpler to work with the one-sided distribution $n_{2R}(1,2)$, in which $n_{2R}(1,2) = 0$ if $x_2 < x_1$, and this is what we shall do. To start, we see that (2.5) is to be replaced by

$$n_{2R,N}(1,2)Q_N = \sum_{\substack{i-j\leq N \\ i,j\geq 1}} \langle J|(ew)^{i-1}|1\rangle\langle 1|(ew)^j|2\rangle\langle 2|(ew)^{N-i-j}e|J\rangle \tag{4.1}$$

and hence (2.8) by

$$n_{2R}(1,2)\Xi = \langle J|(I-zw)^{-1}|1\rangle z(1)\langle 1|w(I-zw)^{-1}|2\rangle z(2)\langle 2|(I-wz)^{-1}|J\rangle. \tag{4.2}$$

Using (2.7), then

$$\langle 1|n_{2R}n^{-1}|2\rangle = \langle (I-zw)^{-1}|1\rangle\langle 1|zw(I-zw)^{-1}|2\rangle / \langle (I-zw)^{-1}|2\rangle \tag{4.3}$$

and it follows at once from (2.9) that

$$n_{2R}n^{-1} = \bar{n}_2 n^{-1}(I-\bar{n}_2 n^{-1})^{-1} \tag{4.4}$$

or conversely

$$\bar{n}_2 n^{-1} = n_{2R}n^{-1}(I+n_{2R}n^{-1})^{-1}. \tag{4.5}$$

We may pause to obtain the direct correlation function in the $\bar{n}_2$ notation. Since

$$n_{2R} = \bar{n}_2(I-n^{-1}\bar{n}_2)^{-1} \tag{4.6}$$

the full density–density expectation is readily seen to reduce to

$$n + n_{2R} + n_{2R}^{\mathrm{T}} = (I-\bar{n}_2^{\mathrm{T}}n^{-1})^{-1}(n-\bar{n}_2^{\mathrm{T}}n^{-1}\bar{n}_2)(I-n^{-1}\bar{n}_2)^{-1} \tag{4.7}$$

where superscript T indicates transpose. However, quite generally

$$(A-vv^{\mathrm{T}})^{-1} = A^{-1} + (A^{-1}v)(v^{\mathrm{T}}A^{-1})/(1-v^{\mathrm{T}}A^{-1}v) \tag{4.8}$$

and one recalls the alternative representation for the complete direct correlation function

$$C = (n + n_2 - \boldsymbol{n}\boldsymbol{n}^{\mathrm{T}})^{-1} \tag{4.9}$$

where $\boldsymbol{n}$ is a vector. We conclude from (4.7)–(4.9) that

$$C(1,2) = \frac{1}{n(1)n(2)}\left(\langle 1|B|2\rangle + \frac{\langle 1|B\rangle\langle B|2\rangle}{1-\langle B\rangle}\right) \tag{4.10}$$

where $B = (n-\bar{n}_2^{\mathrm{T}})(n-\bar{n}_2^{\mathrm{T}}n^{-1}\bar{n}_2)^{-1}(n-\bar{n}_2)$.

Now, continuing with our transcription, we have, from (4.5),

$$\bar{n}_2 = n_{2R}(n+n_{2R})^{-1}n = n(n+n_{2R})^{-1}n_{2R} \tag{4.11}$$

so that

$$n(1) - \int \bar{n}_{2R}(1,2)\,\mathrm{d}2 = n(1)\langle 1|(n+n_{2R})^{-1}n\rangle \tag{4.12a}$$

$$n(1) - \int \bar{n}_{2R}(2,1)\,\mathrm{d}2 = \langle n(n+n_{2R})^{-1}|1\rangle n(1). \tag{4.12b}$$

Thus the entropy of (2.21) becomes

$$
\begin{aligned}
-S/\kappa = & \int\int \langle 1|n_{2R}(n+n_{2R})^{-1}n|2\rangle \ln\langle 1|n_{2R}(n+n_{2R})^{-1}n|2\rangle \, \mathrm{d}1\, \mathrm{d}2 \\
& + \int \langle 1|n(n+n_{2R})^{-1}n\rangle \ln\langle 1|n(n+n_{2R})^{-1}n\rangle \, \mathrm{d}1 \\
& + \int \langle n(n+n_{2R})^{-1}n|1\rangle \ln\langle n(n+n_{2R})^{-1}n|1\rangle \, \mathrm{d}1 - \int n(1)\ln n(1)\, \mathrm{d}1 \\
& + [1-\langle n(n+n_{2R})^{-1}n\rangle]\ln[1-\langle n|(n+n_{2R})^{-1}n\rangle]. \qquad (4.13)
\end{aligned}
$$

Since $\int\int n_{2R}(1,2)\phi(1,2)\,\mathrm{d}1\,\mathrm{d}2 = \int\int \bar{n}_2(1,2)\phi(1,2)\,\mathrm{d}1\,\mathrm{d}2$ for physical nearest-neighbour potentials, one might imagine that $\beta(u(1)-\mu)$ and $\beta\phi(1,2)$ could again be recovered by differentiating with respect to n and n_{2R}. However, the class of n_{2R} thus represented is severely restricted, and so this is not the case. For example, one readily finds, from (4.13), that

$$
\begin{aligned}
\delta(S/\kappa)/\delta n(1) = & \ln n(1) - \ln\langle 1|n(n+n_{2R})^{-1}n\rangle - \ln\langle n(n+n_{2R})^{-1}|1\rangle \\
& + \ln[1-\langle n(n+n_{2R})^{-1}n\rangle] + R(1) \qquad (4.14)
\end{aligned}
$$

where

$$
\begin{aligned}
R(1) = & -\int\int \langle 2|n_{2R}(n+n_{2R})^{-1}|1\rangle\langle 1|(n+n_{2R})^{-1}n_{2R}|3\rangle \ln\langle 2|n_{2R}(n+n_{2R})^{-1}n|3\rangle \, \mathrm{d}2\, \mathrm{d}3 \\
& + \int \langle 2|(n+n_{2R})^{-1}n_{2R}|1\rangle\langle 1|n_{2R}(n+n_{2R})^{-1}\rangle \ln\langle 2|n(n+n_{2R})^{-1}n\rangle \, \mathrm{d}2 \\
& + \int \langle (n+n_{2R})^{-1}n_{2R}|1\rangle\langle 1|n_{2R}(n+n_{2R})^{-1}|2\rangle \ln\langle n(n+n_{2R})^{-1}n|2\rangle \, \mathrm{d}2 \\
& - \langle (n+n_{2R})^{-1}n_{2R}|1\rangle\langle 1|n_{2R}(n+n_{2R})^{-1}\rangle \ln[1-\langle n_{2R}(n+n_{2R})^{-1}n\rangle] \qquad (4.15)
\end{aligned}
$$

and the remainder $R(1)$ destroys the identity between (4.14) and (2.22).

5. The truncated distribution

In deriving (2.21), use was made only of the nearest-neighbour property of the interaction, since this allows the nearest-neighbour pair distribution to be sampled by perturbing the potential, and vice versa. As we have seen, extending this argument to the full (right) pair distribution will not do for physical range-restricted nearest-neighbour interactions, because an arbitrary full distribution is not produced by this class. Conversely, since a physically consistent nearest-neighbour interaction for cores of diameter a is restricted (unless mediated by excitations of the medium beween two successive particles) to have a range of $2a$, only the truncated distribution

$$\langle 1|\hat{n}_2|2\rangle = \langle 1|\bar{n}_2|2\rangle\epsilon(1+2a-2) \qquad (5.1)$$

is sampled by the interaction. Thus, we should be able to express all quantities in terms of $\hat{n}_2$ and n. To start with, we must write $\bar{n}_2$ in terms of $\hat{n}_2$, and this is not a trivial undertaking. The reverse is trivial: we write (2.20) in the form

$$\langle 1|\bar{n}_2|2\rangle = \exp(-\beta\phi(1,2))\,\frac{\langle 1|n-\bar{n}_2\rangle\langle n-\bar{n}_2|2\rangle}{1-\langle n-\bar{n}_2\rangle} \qquad (5.2)$$

and combine (5.1) for $2-1<2a$ with (5.2) for $2-1\geq 2a$ where $\phi(1,2)=0$, to obtain

$$\langle 1|\bar{n}_2|2\rangle = \langle 1|\hat{n}_2|2\rangle + \frac{\langle 1|n-\bar{n}_2\rangle\langle n-\bar{n}_2|2\rangle}{1-\langle n-\bar{n}_2\rangle}\epsilon(2-1-2a). \tag{5.3}$$

Equation(5.3) is then to be solved for $\bar{n}_2$.

Let us rewrite (5.3) as

$$\langle 1|g|2\rangle = \langle 1|f|2\rangle - \langle 1|g\rangle\langle g|2\rangle\epsilon(2-1-2a) \tag{5.4}$$

where $g\equiv (n-\bar{n}_2)/(1-\langle n-\bar{n}_2\rangle)$, $f\equiv (n-\hat{n}_2)/(1-\langle n-\bar{n}_2\rangle)$. Integrating over 2, and over 1, yields respectively

$$\left(1+\int_{1+2a}^{\infty}\langle g|2\rangle \,\mathrm{d}2\right)\langle 1|g\rangle = \langle 1|f\rangle \tag{5.5a}$$

$$\left(1+\int_{-\infty}^{2-2a}\langle 1|g\rangle \,\mathrm{d}1\right)\langle g|2\rangle = \langle f|2\rangle \tag{5.5b}$$

and hence setting

$$\langle 1|h\rangle = \langle 1|f\rangle/\langle 1|g\rangle \qquad \langle h|1\rangle = \langle f|1\rangle/\langle g|1\rangle \tag{5.6}$$

we have on differentiation

$$\langle f|1+2a\rangle/\langle h|1+2a\rangle = -\langle 1|h\rangle' \tag{5.7a}$$

$$\langle 2-2a|f\rangle/\langle 2-2a|h\rangle = \langle h|2\rangle'. \tag{5.7b}$$

It follows that

$$\langle 1|f\rangle - \langle f|1+2a\rangle = (\langle h|1+2a\rangle\langle 1|h\rangle)' \tag{5.8}$$

so that

$$\langle h|1+2a\rangle\langle 1|h\rangle = c + \int_{-\infty}^{1}(\langle 2|f\rangle - \langle f|2+2a\rangle)\,\mathrm{d}2 \tag{5.9}$$

for a suitable constant c. From (5.7a) and (5.9), then

$$\frac{\langle 1|h\rangle'}{\langle 1|h\rangle} = \frac{\langle f|1+2a\rangle}{c+\int_{-\infty}^{1}(\langle 2|f\rangle - \langle f|2+2a\rangle)\,\mathrm{d}2)} \tag{5.10}$$

or

$$\langle 1|h\rangle = c'\exp\left(-\int_{-\infty}^{1}\frac{\langle f|2+2a\rangle}{c+\int_{-\infty}^{2}(\langle 3|f\rangle - \langle f|3+2a\rangle)\,\mathrm{d}3}\,\mathrm{d}2\right) \tag{5.11}$$

for some constant c'. Then from (5.9), we have as well

$$\langle h|1+2a\rangle = \frac{1}{c'}\left(c + \int_{-\infty}^{1} (\langle 2|f\rangle - \langle f|2+2a\rangle)\,\mathrm{d}2\right) \times \exp\left(\int_{-\infty}^{1} \frac{\langle f|2+2a\rangle}{c+\int_{-\infty}^{2}(\langle 3|f\rangle - \langle f|3+2a\rangle)\,\mathrm{d}3}\,\mathrm{d}2\right). \tag{5.12}$$

To evaluate the parameters c and c' in (5.11) and (5.12), we observe from (5.5a) and (5.5b) that $\langle\infty|h\rangle = 1$, $\langle h|-\infty\rangle = 1$. According to (5.12), then, $c' = c$ and, from (5.11), c satisfies

$$c = \exp\left(\int_{-\infty}^{\infty} \frac{\langle f|2+2a\rangle}{c+\int_{-\infty}^{2}(\langle 3|f\rangle - \langle f|2+2a\rangle)\,\mathrm{d}3}\,\mathrm{d}2\right). \tag{5.13}$$

We conclude from (5.11) and (5.12) that

$$\langle 1|g\rangle = \langle 1|f\rangle \exp\left(-\int_{1}^{\infty} \frac{\langle f|2+2a\rangle}{c+\int_{-\infty}^{2}(\langle 3|f\rangle - \langle f|3+2a\rangle)\,\mathrm{d}3}\,\mathrm{d}2\right) \tag{5.14a}$$

$$\langle g|1\rangle = \frac{\langle f|1\rangle}{c+\int_{-\infty}^{1}(\langle 2-2a|f\rangle - \langle f|2\rangle)\,\mathrm{d}2} \times \exp\left(\int_{1}^{\infty} \frac{\langle f|2\rangle}{c+\int_{-\infty}^{2}(\langle 3-2a|f\rangle - \langle f|3\rangle)\,\mathrm{d}3}\,\mathrm{d}2\right). \tag{5.14b}$$

In order to convert these to an expression for $n-\bar{n}_2$ in terms of $n-\hat{n}_2$, first integrate (5.14b), an obvious perfect derivative, over 1 from $-\infty$ to ∞, using (5.13) and the definition (5.4), $\langle n-\bar{n}_2\rangle/(1-\langle n-\bar{n}_2\rangle) = c-1$, so that

$$c = \frac{1}{1-\langle n-\bar{n}_2\rangle}. \tag{5.15}$$

We thus have at once

$$\langle 1|n-\bar{n}_2\rangle = \langle 1|n-\hat{n}_2\rangle \exp\left(-\int_{1}^{\infty} \frac{\langle n-\hat{n}_2|2+2a\rangle}{1+\int_{-\infty}^{2}(\langle 3|n-\hat{n}_2\rangle - \langle n-\hat{n}_2|3+2a\rangle)\,\mathrm{d}3}\,\mathrm{d}2\right) \tag{5.16}$$

and

$$\langle n-\bar{n}_2|1\rangle = \frac{\langle n-\hat{n}_2|1\rangle}{1+\int_{-\infty}^{1}(\langle 2-2a|n-\hat{n}_2\rangle - \langle n-\hat{n}_2|2\rangle)\,\mathrm{d}2} \times \exp\left(-\int_{-\infty}^{1} \frac{\langle n-\hat{n}_2|2\rangle}{1+\int_{-\infty}^{2}(\langle 3-2a|f\rangle - \langle f|3\rangle)\,\mathrm{d}3}\,\mathrm{d}2\right) \tag{5.17}$$

as well as

$$c = \exp\left(\int_{-\infty}^{\infty} \frac{\langle n-\hat{n}_2|2+2a\rangle}{1+\int_{-\infty}^{2}(\langle 3|n-\hat{n}_2\rangle - \langle n-\hat{n}_2|3+2a\rangle)\,\mathrm{d}3}\,\mathrm{d}2\right). \tag{5.18}$$

Using the identity

$$1+\int_{-\infty}^{1}(\langle 2-2a|n-\hat{n}_2\rangle-\langle n-\hat{n}_2|2\rangle)\,\mathrm{d}2 = \exp\left(\int_{-\infty}^{1}\frac{\langle 2-2a|n-\hat{n}_2\rangle-\langle n-\hat{n}_2|2\rangle}{1+\int_{-\infty}^{1}(\langle 3-2a|n-\hat{n}_2\rangle-\langle n-\hat{n}_2|3\rangle)\,\mathrm{d}3}\,\mathrm{d}2\right) \tag{5.19}$$

equation (5.17) transforms to the simpler

$$\langle n-\bar{n}_2|1\rangle=\langle n-\hat{n}_2|1\rangle\exp\left(-\int_{-\infty}^{1}\frac{\langle 2-2a|n-\hat{n}_2\rangle}{1+\int_{-\infty}^{2}(\langle 3-2a|n-\hat{n}_2\rangle-\langle n-\hat{n}_2|3\rangle)\,\mathrm{d}3}\,\mathrm{d}2\right) \tag{5.17'}$$

and (5.3) thereby reduces to the desired

$$\begin{aligned}\langle 1|\bar{n}_2|2\rangle=\langle 1|\hat{n}_2|2\rangle+\epsilon(2-1-2a)\langle 1|n-\hat{n}_2|2\rangle&\\ \times\exp\bigg(\int_{-\infty}^{1}\frac{\langle n-\hat{n}_2|3+2a\rangle}{1+\int_{-\infty}^{3}(\langle 4|n-\hat{n}_2\rangle-\langle n-\hat{n}_2|4+2a\rangle)\,\mathrm{d}4}\,\mathrm{d}3&\\ -\int_{-\infty}^{2}\frac{\langle 3-2a|n-\hat{n}_2\rangle}{1+\int_{-\infty}^{3}(\langle 4-2a|n-\hat{n}_2\rangle-\langle n-\hat{n}_2|4\rangle)\,\mathrm{d}4}\,\mathrm{d}3\bigg).&\end{aligned} \tag{5.20}$$

Although the entropy is rather complicated when expressed in terms of $\hat{n}_2$, substitution into (2.19) and (2.20) gives reasonably simple, although not fully transparent, profile equations:

$$\begin{aligned}\beta(\mu-u(1))=\ln\langle n-\hat{n}_2|1\rangle+\ln\langle 1|n-\hat{n}_2\rangle-\ln n(1)&\\ +\int_{-\infty}^{1}\frac{\langle n-\hat{n}_2|2+2a\rangle}{1+\int_{-\infty}^{2}\langle 3|n-\hat{n}_2\rangle-\langle n-\hat{n}_2|3+2a\rangle\,\mathrm{d}3}\,\mathrm{d}2&\\ -\int_{-\infty}^{1}\frac{\langle 2-2a|n-\hat{n}_2\rangle}{1+\int_{-\infty}^{2}\langle 3-2a|n-\hat{n}_2\rangle-\langle n-\hat{n}_2|3\rangle\,\mathrm{d}3}\,\mathrm{d}2&\end{aligned} \tag{5.21}$$

$$\begin{aligned}\exp(-\beta\phi(1,2))=\epsilon(2-1-2a)+\frac{\langle 1|\hat{n}_2|2\rangle}{\langle 1|n-\hat{n}_2\rangle\langle n-\hat{n}_2|2\rangle}&\\ \times\exp\bigg(\int_{-\infty}^{2}\frac{\langle 3-2a|n-\hat{n}_2\rangle}{1+\int_{-\infty}^{3}\langle 4-2a|n-\hat{n}_2\rangle-\langle n-\hat{n}_2|4\rangle\,\mathrm{d}4}\,\mathrm{d}3&\\ -\int_{-\infty}^{1}\frac{\langle n-\hat{n}_2|3+2a\rangle}{1+\int_{-\infty}^{3}\langle 4|n-\hat{n}_2\rangle-\langle n-\hat{n}_2|4+2a\rangle\,\mathrm{d}4}\,\mathrm{d}3\bigg).&\end{aligned} \tag{5.22}$$

6. Conclusions

For a non-uniform pair-interacting system, the external and internal potentials control the one- and two-body densities. An inverse viewpoint is obtained by asking how the one- and two-body densities control the required external and internal potentials, and by Legendre transforming the generating function appropriately. Expressed in this way, nearest-neighbour interactions in one dimension create an explicitly solvable system, with a very simple direct correlation structure. If the interaction is not medium mediated, the nearest-neighbour property requires a pair interaction with hard core and short-range tail, and consequently samples only a limited portion of pair distribution space. However, it is not difficult to have the corresponding pair density as controlling function, and we have carried this out, after doing the same for the full one-sided pair density as a cautionary note. The resulting external and internal profile equations are not complicated and suggest extrapolations to more realistic interactions, which are the subject of current investigations.

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