# Some applications of the Lambert W function to classical statistical mechanics

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# Some applications of the Lambert W function to classical statistical mechanics

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**Abstract**
We apply the recently defined Lambert W function to some problems of
classical statistical mechanics, i.e. the Tonks gas and a fluid of classical particles
interacting via repulsive pair potentials. The latter case is considered both from
the point of view of the standard theory of liquids and in the framework of a
field theoretical description. Some new mathematical properties of the Lambert
W function are obtained by passing.

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## 1. Introduction

The Lambert W function is defined as the multivalued inverse of the function $w \mapsto w\,\mathrm{e}^w$. Its
mathematical properties have been explored only quite recently after its implementation in
the mathematical library of the computer algebra program *Maple*. The history, applications
and properties of Lambert W are reviewed in Corless *et al* [1]. Mathematical developments
and applications to physics (mainly in quantum mechanics and electrostatics) can be found in
[1–4]. Since W is a very simple function, all its applications to physics or other fields are not
exhausted, and, after a short enquiry, I have discovered that many of my colleagues, aware or
unaware of its name, have met the function in their own works [5–7].

Here we reformulate some old and new problems of the statistical mechanics of classical
liquids in terms of Lambert W.

Our paper is organized as follows. In section 2 we commence by refreshing the reader ideas
with some known mathematical properties of $W(z)$. We focus on the principal branch $W_0(z)$ of
the Lambert function and the related function $U_0(z) = W_0(z) + W_0^2(z)/2$, both being of prime
importance for their applications to the problems of statistical mechanics considered in this
paper. Some new mathematical properties of $W_0(z)$ and $U_0(z)$ used in the paper are presented
in the appendix (the Legendre transforms of the real functions $x \in \mathbb{R}$, $x \mapsto W_0(\exp(x))$ and
$x \mapsto U_0(\exp(x))$ are computed and the dispersion relations for $W_0(z)$ and $U_0(z)$ established).

In section 3 we reformulate the properties of the Tonks gas [8], i.e. a one-dimensional (1D) classical fluid of hard rods, in terms of the principal branch $W_0(z)$ of the Lambert function. Our presentation is compared with the seminal work of Hauge and Hemmer on this system [9]. The introduction of Lambert $W_0(z)$ allows to recover all the properties of the model in a unified treatment.

In section 4 we focus on the second system considered by Hauge and Hemmer in [9], i.e. a classical 3D fluid made of particles with intermolecular pair repulsions of the form

$$\varphi(r) = \gamma^3 \phi(\gamma r) \tag{1.1}$$

where $\phi$ is a positive integrable function. The extension to arbitrary dimension is trivial. In the limit $\gamma \to 0$ which will be considered, we deal with infinitely weak and infinitely long-range repulsive interactions. Once again, the use of the functions $W_0(z)$ and $U_0(z)$ is of great help for describing in a unified manner all the known properties of this model.

Section 5 contains new material. We consider the field theoretical representation of a fluid of particles interacting via repulsive potentials in the framework of the formalism developed in [10]. It is shown that at the mean-field (MF) level of the theory the expressions for the pressure and the density are identical to those derived in section 4 for the fluid with weak long-range repulsive interactions. In other words, the MF approximation is exact in the case of infinitely long-range interactions, a satisfactory, although expected result. We conclude in section 6.

## 2. A digest on Lambert W

In this section we summarize the main mathematical properties of the Lambert $W(z)$ function. $W(z)$ is defined as the root of

$$W(z)\, e^{W(z)} = z \tag{2.1}$$

where $z$ is a complex number. For a given $z$, equation (2.1) has an infinite number of solutions and thus $W(z)$ is a multivalued function. Its properties have been studied recently in [1–4]. The different branches of Lambert W (i.e. the different possible solutions of equation (2.1)) are labelled by an integer $k = 0, \pm 1, \pm 2$, etc. When $z$ is a real number equation (2.1) can have either two real solutions for $0 > z > -\exp(-1)$, in which case they are $W_0(z)$ and $W_{-1}(z)$, or it can have only one real solution for $z \geqslant 0$, this being $W_0(z)$ while $W_{-1}(z)$ is now complex, or no real solutions for $-\infty < z < -\exp(-1)$. $W_0(z)$ and $W_{-1}(z)$ are the only branches of $W$ that take on real values.

A brief survey of the properties of the principal branch $W_0(z)$ will be sufficient for our purpose. Firstly, $W_0(z)$ is analytic at $z = 0$. This follows from the Lagrange inversion theorem [11]. Its power series about the point $z = 0$ reads as

$$W_0(z) = \sum_{n=1}^{\infty} \frac{(-n)^{n-1}}{n!} z^n. \tag{2.2}$$

The radius of convergence of the series (2.2) is equal to $e^{-1}$ as it is easily shown using the Cauchy test and, within the circle of convergence, $|W(z)| < 1$. As a consequence of the relation (2.1) one has

$$W_0'(z) = \frac{W_0(z)}{z(1 + W_0(z))} \tag{2.3a}$$

$$= \sum_{n=1}^{\infty} \frac{(-n)^{n-1}}{(n-1)!} z^{n-1} \tag{2.3b}$$

where the radius of convergence of the series (2.3*b*) is again equal to $e^{-1}$. Lagrange theorem gives more than equation (2.2); it allows us to obtain power series for $W_0^\alpha(z)$, $1/(1 + W_0(z))$, $\exp(\alpha W_0(z))$, etc for $z$ within the circle of convergence of $W_0(z)$ [3]. In particular, the power series of the function $U_0(z)$ defined to be $W_0(z) + W_0(z)^2/2$ is given by

$$U_0(z) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1} n^{n-2}}{n!} z^n \quad (|z| < e^{-1}). \tag{2.4}$$

Note that it follows from equation (2.3*a*) that

$$z U_0'(z) = W_0(z). \tag{2.5}$$

$W_0(z)$ has a second-order branch point at $z = -e^{-1}$ which it shares with both $W_1(z)$ and $W_{-1}(z)$ and its branch cut is conveniently chosen to be $\{z : -\infty < z \leqslant -e^{-1}\}$ with the convention that $W_0(z)$ is defined on the upper lip of the branch cut. The behaviour of $W_0(z)$ about the branch point is given by the series [1]

$$W_0(z) = -1 + p - \tfrac{1}{3} p^2 + \tfrac{11}{72} p^3 + \cdots \tag{2.6}$$

where $p = \sqrt{(2(ez + 1)}$ (the series converges for $|p| < \sqrt{2}$).

In physics, it is quite common (and sometimes enlightening) to write dispersion relations for functions having a branch cut such that $W_0(z)$ and $U_0(z)$ [12]. We show in the appendix that, in the present case, these relations can be recast under the form

$$W(U)_0(z) = \int_{-\infty}^{-e^{-1}} g_{W(U)}(s) \ln\left(1 - \frac{z}{s}\right) ds \tag{2.7a}$$

$$g_{W(U)}(s) = -\frac{1}{\pi} \frac{d}{ds} \text{Im}[W(U)(s)] \tag{2.7b}$$

where $z$ is an arbitrary complex number which however is *not* on the branch cut. These equations convey the interpretation of $W_0(z)$ (resp. $U_0(z)$) as the two-dimensional complex electric potential created by a distribution of charges $g_W(s)$ (resp. $g_U(s)$) located on the branch cut. Moreover, we show in the appendix that the distribution $g_W(s)$ is normalized to unity (cf equation (A.14)) while the total charge of the charge distribution $g_U(s)$ is infinite. Other physical interpretations of the relations (2.7) will be discussed in forthcoming developments.

## 3. The Tonks gas

In this section we consider the Tonks gas, i.e. a 1D fluid of hard rods of length $\sigma$ [8]. The equation of state (EOS) is known exactly:

$$\chi \equiv \beta P = \frac{\rho}{1 - \rho\sigma} \tag{3.1}$$

($P$ pressure, $\beta = 1/kT$, $T$ temperature, $\rho$ number density). Of course $0 < \rho\sigma < 1$. For $\rho\sigma \to 0$ one recovers the EOS of the ideal gas, while for $\rho\sigma \to 1$, which corresponds to the close packing of the hard rods, the pressure diverges. Less trivial is the expression of the pressure as a function of the activity $z$. Recall that $z = \exp(\beta\mu)$ where $\mu$ is the chemical potential and we have assumed that the deBroglie thermal wavelength $\Lambda = 1$. Starting from the thermodynamic relation [13]

$$\rho = z \frac{d}{dz} \chi \tag{3.2}$$

it is not difficult to obtain the relation [9]

$$\sigma \chi \, e^{\sigma \chi} = \sigma z. \tag{3.3}$$

*A priori* equation (3.3) is valid only for real positive values of $z$ but it allows us to define the pressure $\chi(z)$ in the complex plane of the activities by analytic continuation. The authors of [9] did not know the Lambert function as we do; clearly one has

$$\chi(z) = \frac{1}{\sigma} W_0(\sigma z) \tag{3.4}$$

since the other branches $W_k$ of Lambert W will not give a real pressure for real chemical potentials $\mu$. The Mayer expansions for the pressure and the density of the Tonks gas are therefore obtained by copying out equations (2.2) and (2.3b):

$$\chi(z) = \sum_{n=1}^{\infty} b_n z^n \tag{3.5a}$$

$$\rho(z) = \frac{1}{\sigma} \frac{W_0(\sigma z)}{1 + W_0(\sigma z)} = \sum_{n=1}^{\infty} n b_n z^n \tag{3.5b}$$

$$b_n = \frac{(-n\sigma)^{n-1}}{n!}. \tag{3.5c}$$

The results of section 2 on Lambert W enable us to conclude that

1. The radius of convergence of the Mayer series (3.5a) and (3.5b) is $R = 1/e\sigma$. Within the circle of convergence $|\chi(z)| < \sigma^{-1}$.
2. The pressure $\chi(z)$ is singular at the point $z = -R$ of the circle of convergence, i.e. the branch point of $W_0(\sigma z)$, in agreement with one of the conclusions of the second theorem of Groeneveld [14].
3. $\chi(z)$ has a branch cut on the negative real axis: $-\infty < s \leqslant -R$. It can be identified with the distribution of zeros of the grand partition function in the thermodynamic limit [15, 16]. The distribution of the Yang–Lee zeros is given by $g(s) = g_W(\sigma s) = -\text{Im } W_0'(\sigma s)/\pi$ (cf equations (2.7a) and (A.13a)). $g(s)$ is a positive and increasing function over the interval $-\infty < s < -R$ which behaves as $g(s) \sim -1/(\sigma s \ln|s|)^2)$ for $s \to -\infty$ and as $g(s) \sim \sqrt{e/2}/(\pi x^{1/2})$ for $x = -R - x$, $x \to 0+$; therefore the integral of $g(s)$ over the interval $-\infty < s < -R$ is convergent and equal to $\sigma$ (cf equation (A.14)).
4. For an arbitrary $z$ (however *not* on the branch cut) the pressure $\chi(z)$ may be seen as the 2D complex electrostatic potential created by the charge distribution $g(s)$. It follows from equations (2.7a) and (A.13a) that $\chi(z)$ takes the form proposed by Yang and Lee [15, 16],

$$\chi(z) = \int_{-\infty}^{-R} g(s) \ln\left(1 - \frac{z}{s}\right) ds \quad (\forall z \text{ not on the cut } -\infty < s \leqslant -R). \tag{3.6}$$

A close examination of their paper reveals that the derivation of equation (3.6) given by Hauge and Hemmer is restricted to a point $z$ inside the circle of convergence.

It is amusing to check the various conclusions of second theorem of Groeneveld [14]. Recall that for a $d$-dimensional classical fluid of particles interacting via positive pair potentials $\varphi(r_{ij}) \geqslant 0$ such that (twice) the second virial coefficient

$$f = \int d^d\vec{r}(\exp(-\beta\varphi(r)) - 1) \tag{3.7}$$

converges, the radius of convergence $R$ of the virial series (3.5a) and the Mayer coefficients $b_n$ satisfy the following inequalities:

$$\frac{1}{e|f|} \leqslant R \leqslant \frac{1}{|f|} \tag{3.8a}$$

$$\frac{1}{n} \leqslant \frac{b_n}{f^{n-1}} \leqslant \frac{n^{n-2}}{n!}. \tag{3.8b}$$

In the present case $f = 2b_2 = -\sigma$, and one easily checks that $R = 1/e\sigma$ and $b_n$ as given by equation (3.5c), do satisfy the Groeneveld inequalities (3.8).

We end this section by determining the Helmholtz free energy per unit volume $\beta f(\rho)$ as the Legendre transform of $\beta P$ viewed as a function of the reduced chemical potential $\nu \equiv \beta\mu = \ln z$ (see e.g. [17]). It follows from equation (A.5) of the appendix that

$$\beta f(\rho) = \sup_{\nu \in \mathbb{R}}(\nu\rho - \chi(e^\nu))$$
$$= \rho(\ln \rho\Lambda - 1) - \rho \ln(1 - \rho\sigma). \tag{3.9}$$

Note that we have restored $\Lambda$ to make the argument of the ln dimensionless. $\beta f(\rho)$ is a strictly convex function of the density defined for $0 < \rho\sigma < 1$. The first term on the RHS of the equation is the Helmholtz free energy per unit volume of the ideal gas while the second one is the excess free energy. The analytic continuation of $\beta f(\rho)$ to complex densities is obtained by defining $\beta f(\rho)$ according to equation (3.9) where ln is the principal branch of the natural logarithm for $\beta f(\rho)$ must take on real values for $\rho \in \mathbb{R}, 0 < \rho\sigma < 1$. $\beta f(\rho)$ is then a multivalued function with two branch cuts $-\infty < \rho \leqslant 0$ and $\sigma^{-1} \leqslant \rho < +\infty$.

## 4. Weak- and long-range repulsion

The EOS of a gas of particles interacting via the pair potential (1.1) is known exactly and given by [9]

$$\chi \equiv \beta P = \rho + \frac{a}{2}\rho^2 \tag{4.1}$$

where

$$a = \beta\tilde{\phi}(0) \equiv \int d^3\vec{r} \, \beta\phi(r) \tag{4.2}$$

is a positive, $\gamma$-independent constant. Here $\rho$ can take on all non-negative real values. It is not difficult to obtain the relation between the density and the activity which reads as [9]

$$z = \rho \, e^{a\rho}. \tag{4.3}$$

Therefore, since for a real $z$ the density must be real

$$\rho = \frac{1}{a}W_0(az) \tag{4.4}$$

and, by integration of the thermodynamic relation (3.2)

$$\chi(z) = \frac{1}{a}U_0(az). \tag{4.5}$$

The pressure and the density for complex activities are obtained by analytical continuations of equations (4.4) and (4.5). The virial series for $\chi(z)$ and $\rho(z)$ follow from equations (2.2) and (2.4),

$$\chi(z) = \sum_{n=1}^{\infty} \frac{(-a)^{n-1}n^{n-2}}{n!}z^n \tag{4.6a}$$

$$\rho(z) = \sum_{n=1}^{\infty} \frac{(-a)^{n-1}n^{n-1}}{n!}z^n. \tag{4.6b}$$

The radius of convergence of these two series is $R = (ae)^{-1}$ and it satisfies the first Groeneveld inequality (3.8a). One also checks that the coefficients of the power series (4.6a) do satisfy the second Groeneveld inequality (3.8b). $\chi(z)$ has a branch cut on the negative real axis: $-\infty < s \leqslant -R$. For any complex activity $z$ *not* on the cut, it can be written once again under the form proposed by Yang and Lee [15, 16] (cf equation (A.13b)),

$$\chi(z) = \int_{-\infty}^{-R} g(s) \ln\left(1 - \frac{z}{s}\right) ds \tag{4.7}$$

where

$$g(s) = g_U(as) = -\frac{1}{\pi as} \operatorname{Im} W_0(as). \tag{4.8}$$

It follows from the analysis given in the appendix that the function $g(s)$ is not integrable on the cut (it behaves as $-1/as$ for $s \to -\infty$). Recall that, strictly speaking, the theory of Yang and Lee is valid only for interactions with a hard-core contribution. In this case the grand partition function $\Xi$ for a finite volume $V$ is a polynomial in $z$. The distribution $g(s)$ of its zeros after the passage to the thermodynamic limit allows us to rewrite $\chi(z) \equiv \ln \Xi/V$ under the form (4.7), where $g(s)$ is normalizable [9, 15, 16]. For soft interactions as those considered in this section, the reasoning breaks down, leaving us with a non-normalizable distribution $g(s)$ (one can pack an infinite number of particles in a finite volume and the density $\rho$ is not bounded).

Finally the Helmholtz free energy per unit volume $\beta f(\rho)$ is computed as the Legendre transform of $\chi(e^\nu)$. It follows from equation (A.6) of the appendix that

$$\beta f(\rho) = \sup_{\nu \in \mathbb{R}} \left(\nu\rho - \frac{1}{a} U_0(a\, e^\nu)\right)$$

$$= \rho(\ln \rho \Lambda^3 - 1) + \frac{a}{2} \rho^2. \tag{4.9}$$

$\beta f(\rho)$ is a strictly convex function of $\rho$ on the interval $0 < \rho < +\infty$.

## 5. Repulsive interactions: a field theoretical approach

We consider the statistical mechanics of a system made of $N$ classical point particles interacting via pair potentials of the form

$$v(r) = \varphi_0(r) + \varphi(r) \tag{5.1}$$

where $\varphi_0(r)$ is some reference potential (e.g. a hard sphere repulsion for instance) and $\varphi(r)$ admits a positive, well-defined Fourier transform $\tilde{\varphi}(k) \geqslant 0$. $\varphi_0(r)$ and $\varphi(r)$ are supposed to meet all the requirements which are necessary for the existence of a thermodynamic limit (TL) [18].

We denote by $\Omega$ the domain occupied by the molecules of the fluid. It will be convenient to assume that $\Omega$ is a cube of side $L$ with periodic boundary conditions (PBC). In a given configuration $\omega = (N; \vec{r}_1 \ldots \vec{r}_N)$ the microscopic density of particles reads as

$$\hat{\rho}(\vec{r}) = \sum_{i=1}^{N} \delta^{(3)}(\vec{r} - \vec{r}_i) \tag{5.2}$$

and its Fourier transform

$$\hat{\rho}_{\vec{k}} = \sum_{i=1}^{N} \exp(-i\vec{k} \cdot \vec{r}_i). \tag{5.3}$$

The configurational potential energy of the system can be decomposed as

$$\beta V(\omega) = \beta V_0(\omega) - N\nu_S + \frac{\beta}{2}\langle\hat{\rho}|\varphi|\hat{\rho}\rangle \tag{5.4}$$

where $V_0(\omega)$ is the configurational energy of the reference system, $\nu_S \equiv \beta\varphi(0)$ a self-energy contribution and

$$\langle\hat{\rho}|\varphi|\hat{\rho}\rangle \equiv \int_\Omega d^3\vec{r}_1 \, d^3\vec{r}_2 \, \hat{\rho}(\vec{r}_1)\varphi(\vec{r}_1,\vec{r}_2)\hat{\rho}(\vec{r}_2). \tag{5.5}$$

We shall work in the grand canonical (GC) ensemble. We denote by $\mu$ the chemical potential and by $\psi(\vec{r})$ an external potential. The local chemical potential will be noted as $\nu(\vec{r}) = \beta(\mu - \psi(\vec{r}))$. Performing a Kac–Siegert–Stratonovich–Hubbard–Edwards (KSSHE) transform [19–23] one can show that the GC partition function can be recast under the form of a functional integral [10]

$$\Xi[\nu] = \mathcal{N}^{-1}\int \mathcal{D}\xi \exp(-\mathcal{H}[\xi]) \tag{5.6}$$

where $\mathcal{D}\xi$ is the functional measure and the action $\mathcal{H}[\xi]$ of the KSSHE field theory reads as

$$\mathcal{H}[\xi] = \frac{1}{2\beta}\langle\xi|\varphi^{-1}|\xi\rangle - \log\Xi_0[\bar{\nu} + i\xi] \tag{5.7}$$

where $\bar{\nu} = \nu + \nu_S$ and $\Xi_0$ is the GC partition function of the reference system. The field $\xi$ which enter equations (5.6) and (5.7) is a real scalar field. Note that, in the general case where the sign of $\tilde{\varphi}(k)$ is arbitrary, the action $\mathcal{H}$ involves *two* real scalar fields $\xi_+$ and $\xi_-$ (or a complex field $\xi$) [10]. Finally, the normalization constant $\mathcal{N}$ is given by

$$\mathcal{N} = \int \mathcal{D}\xi \exp\left(-\frac{1}{2\beta}\langle\xi|\varphi^{-1}|\xi\rangle\right). \tag{5.8}$$

In [10] the potential $\varphi_0(r)$ of the reference system was chosen to be a hard-core potential of diameter $\sigma$. Here we specialize to the case $\sigma \to 0$ (or equivalently $\varphi_0 \equiv 0$), i.e. we take for the reference system the ideal gas. All the conclusions of [10] remain valid provided that the TL of our system is well behaved. Note that the configuration energy (5.4) can be rewritten as

$$V(\omega) = \frac{1}{L^3}\sum_{\vec{k}}|\hat{\rho}_{\vec{k}}|^2\tilde{\varphi}(k) - \frac{N}{2}\varphi(0). \tag{5.9}$$

Therefore if $\tilde{\varphi}(k) \geqslant 0$ for all $k$ and $\varphi(0) > 0$ (which will be assumed henceforth) then $V(\omega) \geqslant -NB$ with $B(\equiv\varphi(0)/2) > 0$, i.e. the system is H-stable in the sense of Ruelle and the TL exists [18]. Note that, conversely, if $\tilde{\varphi}(k = 0) < 0$, the system does not have a thermodynamic behaviour and the introduction of a repulsive hard core is mandatory to ensure the existence of a TL. Such potentials (i.e. hard core plus an attractive tail) can yield a liquid–vapour transition as explained in [10]; in the case considered here (soft repulsive tail), the possibility of such a transition has to be ruled out.

With the choice $\varphi_0 \equiv 0$ the KSSHE action reads now

$$\mathcal{H}[\xi] = \frac{1}{2\beta}\langle\xi|\varphi^{-1}|\xi\rangle - \int_\Omega d^3\vec{r}\, e^{\bar{\nu}(\vec{r})+i\xi(\vec{r})}. \tag{5.10}$$

We now turn our attention to the mean-field (MF) level of the theory. The MF or saddle-point approximation is defined by the equation

$$\Xi_{MF}(\nu) \equiv \exp(-\mathcal{H}(\bar{\xi})) \tag{5.11}$$

where at $\xi = \bar{\xi}$ the action $\mathcal{H}$ is stationary. The stationary condition

$$\left.\frac{\delta\mathcal{H}}{\delta\xi(\vec{r})}\right|_{\bar{\xi}} = 0 \tag{5.12}$$

can be recast under the form of the implicit integral equation

$$\bar{\xi}(\vec{r}) = i\beta \int_{\Omega} d^3\vec{r}' \, \varphi(\|\vec{r} - \vec{r}'\|) \, e^{\bar{\nu}(\vec{r}') + i\bar{\xi}(\vec{r}')}. \tag{5.13}$$

Moreover the MF density of the fluid is given by the density of the reference fluid—here the ideal gas—at the local chemical potential $\bar{\nu}(\vec{r}) + i\bar{\xi}(\vec{r})$ [10], i.e.

$$\rho_{\mathrm{MF}}(\vec{r}) = e^{\bar{\nu}(\vec{r}) + i\bar{\xi}(\vec{r})}. \tag{5.14}$$

In the case of a homogeneous system to which we stick from now, (i.e. $\psi(\vec{r}) \equiv 0$) the solution of equation (5.13) is a constant $\bar{\xi}$ which is clearly given by

$$\bar{\xi} = i W_k(\lambda z) \tag{5.15}$$

where $W_k$ is some branch of Lambert W, $z$ the activity and

$$\lambda = \beta \tilde{\varphi}(0) \, e^{\nu_S} \tag{5.16}$$

from which it follows that

$$\rho_{\mathrm{MF}} = W_k(\lambda) / \beta \tilde{\varphi}(0). \tag{5.17}$$

It remains to determine the branch of W. For real activities $z$, the MF density should be a positive real number; it follows then from equation (5.17) that, necessarily, $k = 0$. The MF pressure is easily derived from equation (5.11) with the result

$$\chi_{\mathrm{MF}}(z) = \ln \Xi_{\mathrm{MF}} / \Omega$$
$$= \frac{1}{\beta \tilde{\varphi}(0)} U_0(\lambda z). \tag{5.18}$$

Note that the MF equation of state takes the familiar form $\chi_{\mathrm{MF}}(\rho) = \rho + \beta \tilde{\varphi}(0) \rho^2 / 2$. Finally, the MF free energy is obtained by a Legendre transform of $\chi(z)$, which gives

$$\beta f_{\mathrm{MF}} = \rho(\ln(\rho \Lambda^3) - 1) - \rho \nu_S + \beta \tilde{\varphi}(0) \rho^2 / 2 \tag{5.19}$$

in agreement with the general expression of [10].

Some comments are in order.

1. The Taylor series of $\chi_{\mathrm{MF}}(z)$ and $\rho_{\mathrm{MF}}(z)$ in terms of the activity $z$ are once again given by equations (2.2) and (2.4) with a radius of convergence equal to $R = (\lambda e)^{-1}$. For an arbitrary complex activity $z$, the pressure $\chi_{\mathrm{MF}}(z)$ is given by the dispersion relation (4.7).

2. We have shown elsewhere [10] that the one-loop order approximation of the KSSHE field theory coincides with the random phase approximation (RPA) of the theory of liquids [13]. As is well known, for long-range potentials of the form (1.1) the RPA corrections to the pressure vanish as $\gamma \to 0$ [13]. Note that, in this limit, $\nu_S \to 0$ and $\tilde{\varphi}(0) = \tilde{\phi}(0)$; thence, in the limit $\gamma \to 0$, one recovers for the pressure, the free energy etc the expressions derived in section 4. Stated otherwise, the MF-KSSHE theory is exact for infinitely weak and long-range repulsive potentials.

3. We have shown in [10] that the MF pressure and free energy constitute *exact* bounds. More precisely we have

$$\forall z \in \mathbb{R} \qquad \chi(z) \leqslant \chi_{\mathrm{MF}}(z) \equiv U_0(\lambda z) / \beta \tilde{\varphi}(0) \tag{5.20a}$$

$$\forall \rho > 0 \qquad \beta f(\rho) \geqslant \beta f_{\mathrm{MF}}(\rho) \equiv \rho(\ln(\rho \Lambda^3) - 1) - \rho \nu_S + \beta \tilde{\varphi}(0) \rho^2 / 2. \tag{5.20b}$$

## 6. Conclusion

In this paper we have discussed some applications of the Lambert W function to the theory of liquids. In the case of 1D hard rods or infinitely weak long-range repulsive potentials, one obtains a close expression for the complex pressure $\chi(z)$ as a function of complex activities in terms of either $W_0(z)$ or the related function $U_0(z)$. The dispersion relations derived for $W_0(z)$ and $U_0(z)$ in the appendix give a rigorous justification to the heuristic formula proposed by Lee and Yang for $\chi(z)$ [15, 16]. We have also shown that, in the framework of the KSSHE field theory of liquids, the MF pressure $\chi(z)$ of a gas of particles interacting via soft repulsive potentials can be expressed in terms of the function $U_0(z)$.

## Acknowledgments

## Appendix. New mathematical properties of Lambert W

### A.1. Legendre transforms

Let us first consider the real function $x \mapsto f(x) = W_0(e^x)$. By applying twice the formula (2.3a) one finds

$$f'(x) = \frac{f(x)}{1 + f(x)} \tag{A.1a}$$

$$f''(x) = \frac{f(x)}{(1 + f(x))^3}. \tag{A.1b}$$

It follows from equation (A.1b) that $f''(x) > 0$ for all $x \in \mathbb{R}$. Thence the function $f$ is strictly convex and one can define its Legendre transform $\mathcal{L}_f(\rho)$ (see e.g. [17]). By definition

$$\mathcal{L}_f(\rho) = \sup_x (x\rho - f(x)) \tag{A.2}$$

or, more precisely

$$\mathcal{L}_f(\rho) = \bar{x}\rho - f(\bar{x}) \tag{A.3}$$

where $\bar{x}$ is (the unique) solution of

$$\rho = f'(\bar{x}) = \frac{f(\bar{x})}{1 + f(\bar{x})}. \tag{A.4}$$

Therefore $\mathcal{L}_f(\rho)$ is defined for $0 < \rho < 1$. It is also a strictly convex function, the Legendre transform of which is $f(x)$ (i.e. the Legendre transform is involutive). In order to get the expression of $\mathcal{L}_f(\rho)$ one notes that equation (A.4) implies that $f(\bar{x}) = \rho/(1 - \rho)$ and that $\bar{x} = f(\bar{x}) + \ln f(\bar{x})$ which yields

$$\mathcal{L}_f(\rho) = \rho(\ln \rho - 1) - \rho \ln(\rho - 1). \tag{A.5}$$

Similarly it can easily be shown that the function $x \mapsto h(x) = U_0(e^x)$ is strictly convex and that its Legendre transform $\mathcal{L}_h(\rho)$ is given by

$$\mathcal{L}_h(\rho) = \rho(\ln \rho - 1) + \frac{\rho^2}{2}. \tag{A.6}$$

Note that $\mathcal{L}_h(\rho)$ is defined on $0 < \rho < \infty$. Over this interval, $\mathcal{L}_h(\rho)$ is strictly convex.
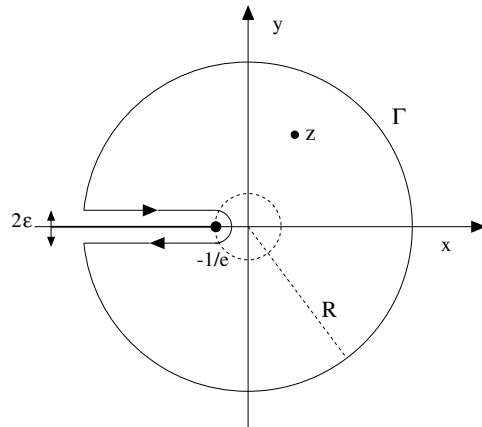
**Figure 1.** Solid line: contour of integration of equation (A.7). The small circle (dashed line) is the circle of convergence of $W_0(z)$ about $z = 0$, the dot is the branch point and the thick solid line is the branch cut. The point $z$ is everywhere except on the cut.

### A.2. Dispersion relations

We establish here the dispersion relations for the functions $W_0(z)$ and $U_0(z)$. Let us first consider $W_0(z)$. It follows from the Cauchy theorem that

$$W_0(z) = \frac{1}{2\pi i} \int_{\mathcal{C}} W_0(s) \left\{ \frac{1}{z-s} - \frac{1}{s} \right\} ds \tag{A.7}$$

where $\mathcal{C}$ is the contour shown in figure 1 and $z$ is *not* on the cut $(-\infty, -e^{-1})$. Indeed $W_0(0) = 0$ as follows from equation (2.2). We consider now equation (A.7) in the limit $\epsilon \to 0$ and $R \to \infty$.

The asymptotic formula for large (complex) $z$, i.e., [1, 4]

$$W_0(z) \sim \ln(z) - \ln(\ln(z)) \tag{A.8}$$

where $\ln z$ is the principal branch of the natural logarithm, ensures that the contribution to equation (A.7) from the large circle $\Gamma$ tends to zero as its radius $R$ tends to infinity (Jordan lemma). Note that we have subtracted $W_0(0) = 0$ from $W_0(z)$ in equation (A.7) precisely in order to obtain this property. Therefore we have

$$W_0(z) = \frac{1}{2\pi i} \int_{-\infty}^{-e^{-1}} \left\{ W_0(s + i\epsilon) \left[ \frac{1}{s + i\epsilon - z} - \frac{1}{s + i\epsilon} \right] \right.$$
$$\left. - W_0(s - i\epsilon) \left[ \frac{1}{s - i\epsilon - z} - \frac{1}{s - i\epsilon} \right] \right\} ds. \tag{A.9}$$

As $\epsilon \to 0$, we can neglect the $\pm i\epsilon$ in the fractions that enter the RHS of equation (A.9) (remember that $z$ is *not* on the cut) and we get

$$W_0(z) = \frac{1}{2\pi i} \int_{-\infty}^{-e^{-1}} [W_0(s + i\epsilon) - W_0(s - i\epsilon)] \left[ \frac{1}{s-z} - \frac{1}{s} \right] ds. \tag{A.10}$$

With the convention that $W_0(s)$ is defined on the upper lip of the cut and by noting that $W_0(\bar{s}) = \overline{W_0(s)}$ (for $s$ not on the cut) we infer from equation (A.10) that

$$W_0(z) = \frac{1}{\pi} \int_{-\infty}^{-e^{-1}} \mathrm{Im}(W_0(s)) \left[ \frac{1}{s-z} - \frac{1}{s} \right] ds. \tag{A.11}$$

The final step is to perform an integration by parts which yields

$$W_0(z) = \left[\mathrm{Im}(W_0(s)) \ln \left(1 - \frac{z}{s}\right)\right]_{-\infty}^{-e^{-1}} + \int_{-\infty}^{-e^{-1}} \frac{-1}{\pi} \frac{\mathrm{d}}{\mathrm{d}s} \mathrm{Im}(W_0(s)) \ln \left(1 - \frac{z}{s}\right) \mathrm{d}s. \qquad (A.12)$$

Since, in one hand $W_0(-e^{-1}) = -1$ and, on the other hand, $\mathrm{Im}\,(W_0\,(-\infty)) = \pi$ as can be obtained for instance from the asymptotic behaviour (A.8) of $W_0(z)$, then the first contribution to the RHS of equation (A.12) vanishes and we are left with

$$W_0(z) = \int_{-\infty}^{-e^{-1}} g_W(s) \ln \left(1 - \frac{z}{s}\right) \mathrm{d}s \qquad (A.13a)$$

$$g_W(s) = -\frac{1}{\pi} \frac{\mathrm{d}}{\mathrm{d}s} \mathrm{Im}[W_0(s)]. \qquad (A.13b)$$

Several comments are in place here.

(a) The function $g_W(s)$ is a positive increasing function on the cut $(-\infty, -e^{-1})$. For $s = -e^{-1} - x$ ($x \to +0$), $g_W(s) \sim \sqrt{e/2}/(\pi x^{1/2})$ as can be seen from the series expansion of $W_0(z)$ about the branch point (cf equation (2.6)). On the other hand $g_W(s) \sim -1/(s \ln|s|)^2)$ for $s \to -\infty$ as can be inferred from equation (A.8). Thence the integral of $g_W(s)$ along the branch cut is convergent; more precisely

$$\int_{-\infty}^{-e^{-1}} g_W(s)\,\mathrm{d}s = [\mathrm{Im}(W_0(-\infty)) - \mathrm{Im}(W_0(-e^{-1}))]/\pi$$
$$= 1. \qquad (A.14)$$

(b) The dispersion relations for the function $U_0(z)$ are similar to equations (A.13a) for the reasoning presented above can be reproduced without major changes. The distribution $g_U(s)$ is again a positive function on the interval $(-\infty, -e^{-1})$. It is given by

$$g_U(s) = -\pi^{-1} \mathrm{d}(\mathrm{Im}\,U_0(s))/\mathrm{d}s$$
$$= -\frac{\mathrm{Im}\,W_0(s)}{\pi s} \qquad (A.15)$$

from which it follows that $g_U(-e^{-1}) = 0$ because $W_0(-e^{-1}) = -1$. Moreover, for $s \to -\infty$ we have $g_U(s) \sim -1/s$ with the consequence that the integral of $g_U(s)$ along the branch cut is divergent to $+\infty$.

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