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1   The v^μ are the components of the electromagnetic (real) vector field and ψ is the Dirac spinor field; i.e., ψ is a function from space–time into a four-dimensional vector space called spin space. The positive definite inner product in spin space is denoted by $\psi^\dagger\psi$ and $\overline{\psi}$ denotes $\psi^\dagger\gamma^0$. The γ's are operators in spin space which satisfy $\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}(g^{00}=1, g^{ii}=-1, g^{\mu\nu}=0 \; \mu \neq \nu)$ and $\gamma^{0*}=\gamma^0, \gamma^{i*}=-\gamma^i$. All representations of operators satisfying these properties are unitarily equivalent. For this work, as usual, no specific choice is required.

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7   In this work it will be notationally convenient to view the four component spinor ψ as a pair of two component spinors.

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A Functional Equation in the Theory of Fluids*

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Two functional equations of the form $\psi^2(s) - E(s)\phi^2(s) = V(s)$, where s is a complex variable and $E(s)$ and $V(s)$ are given even polynomials, are solved for the even entire functions ψ and ϕ which are required to behave like $\cosh[\alpha s + o(s)]$ for large $|R|s|$. Two cases are considered: (i) V of degree zero and E of degree two and (ii) V of degree eight and E of degree six. In the second case the polynomials must satisfy a condition in order for ψ and ϕ to have the right asymptotic behavior. These functional equations arise in solving the Percus–Yevick equation for a mixture of hard spheres with nonadditive diameters.

1. INTRODUCTION

This is a sequel to the paper by Lebowitz and Zomick.[1] That paper will be referred to below as LZ. The problem considered in it was that of solving the Percus–Yevick (PY) integral equation[2] for a binary mixture of particles in which the two-body interaction potential $u_{ij}(r)$ between a particle of species i and one of species j a distance r apart is given by

$$u_{ij}(r) = \begin{cases} +\infty & (0 \leq r \leq R_{ij}) \\ 0 & (r > R_{ij}) \end{cases}, \quad i, j \in \{1, 2\}, \quad (1.1)$$

where

$$R_{12} = R_{21} = \tfrac{1}{2}(R_{11} + R_{22}) + \alpha,$$
$$\text{with} \quad 0 \leq \alpha \leq \tfrac{1}{2}(R_{22} - R_{11}). \quad (1.2)$$

It was shown by LZ that the solution of the PY equation for this problem involved a functional equation of the form

$$\psi^2(s) - E(s)\phi^2(s) = V(s), \quad (1.3)$$

where s is a complex variable, E and V are polynomial functions of a given form, but with undetermined coefficients, and ϕ and ψ are the unknown functions (related to the Laplace transforms of certain correlation functions), which are required to be even and entire and to satisfy the asymptotic condition

$$\left. \begin{array}{l} \ln|\psi(s)| \\ \ln|\phi(s)| \end{array} \right\} \sim \begin{cases} \alpha R|s & \text{as } R|s \to \infty \\ -\alpha R|s & \text{as } R|s \to -\infty \end{cases}, \quad (1.4)$$

where α is a positive number defined in (1.2).

In the present paper we give a method for solving equations of the form (1) and apply it to the particular equations of this form which arise in LZ. The solution for the particular case which refers to the one-

dimensional hard-rod system with potential (1.1) was quoted, without derivation, in LZ.

The basic idea of the method can be seen by considering the case where $E(s) = V(s) = 1$. Here the equation reduces to

$$\psi(s)^2 - \phi(s)^2 = 1, \quad (1.5)$$

which can be written

$$[\psi(s) + \phi(s)][\psi(s) - \phi(s)] = 1. \quad (1.6)$$

This shows that both $\psi + \phi$ and $\psi - \phi$ are entire functions without zeros and hence must be of the form $\exp[w(s)]$ and $\exp[-w(s)]$, respectively, where w is entire; it follows that the solution is

$$\psi(s) = \cosh w(s), \qquad \phi(s) = \sinh w(s).$$

The method we shall describe is based on the same factorization idea, with modifications to allow for the presence of the polynomials $E(s)$ and $V(s)$ and the conditions that the functions ϕ and ψ must be even and satisfy the asymptotic condition (1.4).

In the next stage of the calculation we shall use the following information about the specific form of the polynomial $E(s)$; it is taken from LZ. The details depend on the number of dimensions of the hard-sphere system.

A. One Dimension

Equation (1.3) above corresponds to Eq. (3.57) of LZ with

$$E(s) = s^2 - 4\mu^2$$
$$\{= D(s)/[(\rho_1 - \rho_2)^2 a^2] \text{ in LZ notation}\}, \quad (1.7)$$

$$V(s) = A, \quad (1.8)$$

where μ and A are positive numbers.

Our $\psi(s)$ and $\phi(s)$ correspond to $\psi(s)$ and $[Q(s)(\rho_1 - \rho_2)a]$ in the notation of LZ.

B. Three Dimensions

Equation (1.3) corresponds to Eq. (5.52) of LZ with

$$E(s) = s^6 - 4h(s), \tag{1.9}$$

$$V(s) = -h(s)A(s), \tag{1.10}$$

where
$$h(s) = h_1 s^2 + h_2 \quad [\text{Eq. (5.38) of LZ}],$$
and
$$A(s) = a_1 s^6 + a_2 s^4 + a_3 s^2 + a_4 \quad [\text{Eq. (5.43) of LZ}].$$

Here $h_1, \ldots, a_4$ are real numbers. This time our $\psi(s)$ and $\phi(s)$ correspond to the $\psi(s)$ and $\phi(s)$ of LZ.

2. FACTORIZATION OF THE EQUATION

To factorize $\psi^2 - E\phi^2$ we define $\sqrt{E(s)}$ to be the branch of the many-valued function $[E(s)]^{1/2}$ which is analytic in the complex s plane with suitable finite cuts, and which satisfies

$$\sqrt{E(s)} \sim s^p \quad \text{for large } s, \tag{2.1}$$

where p is the number of dimensions. This is possible because $E(s) = s^{2p} + \cdots$ both for $p = 1$ and for $p = 3$. Before we proceed, it is worth noting that if the cuts are symmetrical about the origins, as we shall choose them to be, then $\sqrt{E}$ is an odd function of s; for, since E itself is even, the ratio $\sqrt{E(s)}/\sqrt{E(-s)}$ when squared gives 1 and must therefore equal $+1$ or -1 throughout the cut plane, and Eq. (2.1) shows that the value is -1 both for $p = 1$ and for $p = 3$.

We can now factorize the left-hand side of (1.3) by defining

$$f(s) = \psi(s) + \sqrt{E(s)}\phi(s), \tag{2.2}$$

$$\overline{f}(s) = \psi(s) - \sqrt{E(s)}\phi(s) = f(-s) \tag{2.3}$$

since $\sqrt{E}$ is odd and ψ and ϕ are even. Equation (1.3) now becomes

$$f(s)\overline{f}(s) = V(s) \tag{2.4}$$
or
$$f(s)f(-s) = V(s). \tag{2.4'}$$

The behavior of $f(s)$ for large s is determined by the condition (1.4). This condition, with (2.2) and (2.3), gives

$$|\psi(s)| = \tfrac{1}{2}|f(s) + f(-s)| = \exp[\alpha|Rls| + o(s)],$$
$$|Rls| \to \infty, \tag{2.5}$$

so that either $|f(s)|$ or $|f(-s)|$ (or both) grows at least as fast as $\exp[\alpha|Rls| + o(s)]$ as $|Rls| \to \infty$. Suppose for definiteness that it is $f(s)$ that has this property for $Rls \to \infty$; then (2.4) implies that $f(-s)$ decreases exponentially as $Rls \to \infty$ and thus $f(s)$ has to decrease exponentially as $Rls \to -\infty$. Thus we find that in this case

$$|f(s)| \sim \exp[\alpha Rls + o(s)] \quad \text{as } |Rls| \to \infty. \tag{2.6}$$

The alternative possibility gives a similar result, and the two can be combined in the single formula

$$|f(s)| \sim \exp[\pm \alpha Rls + o(s)]$$

as $Rls \to \infty$ *and as* $Rls \to \infty$. $\tag{2.7}$

We also want to know how f behaves on the boundary of the cut plane, i.e., on the cuts themselves. Each cut has two sides which we designate the $+$ and the $-$ side, respectively. If the cut is horizontal, it is convenient to take the $+$ side as the top. We define, for each function F over the cut plane, two boundary-value functions on each cut,

$$F^{\pm}(t) = \lim_{\epsilon \to 0} F(t + \epsilon), \quad t \in C, \tag{2.8}$$

the limit being approached from the $+$ side of the cut C for F^+ and the $-$ side for F^-. For example, since $\sqrt{E}$ reverses sign as we cross any cut, it satisfies

$$\sqrt{E^+}(t) = -\sqrt{E^-}(t) \quad (t \in C) \tag{2.9}$$

Using this in (2.3), we obtain

$$f^+(t) = \overline{f}^-(t) \quad \text{and} \quad \overline{f}^+(t) = f^-(t).$$

It follows, by (2.4), that f satisfies the boundary condition

$$f^+(t)f^-(t) = V(t) \quad (t \in C). \tag{2.10}$$

This equation, together with (2.7), constitutes a boundary-value problem for determining f, of the type discussed by Muskhelishvili.[3] In the following, we shall apply his methods to it.

3. THE ONE-DIMENSIONAL CASE

In this case $V(t)$ is a positive constant A so that the functional equation reduces to

$$f(s)f(-s) = A, \quad s \in \text{cut plane}, \tag{3.1}$$

and (2.10) to

$$f^+(t)f^-(t) = A, \quad t \in [-2\mu, 2\mu]. \tag{3.2}$$

There is just one cut now, since $\sqrt{E(s)} = \sqrt{(s^2 - 4_\mu^2)}$, with two branch points.

We shall write (3.2) in logarithmic form, in terms of

$$\Phi(s) = \ln f(s), \tag{3.3}$$

but it is necessary first to show that $\Phi(s)$ is a (single-valued) function. That is to say, we wish to show that $f(s)$ never vanishes, and that $\arg f(s)$ returns to its original value when s describes any closed contour in the cut plane. Both facts follow from (3.1), the first because $f(-s)$ is holomorphic in the cut plane and the second because any closed contour in the cut plane can be deformed either to zero or to a large circular contour; if it deforms to zero there is no problem, and if not, both s and $-s$ traverse the same circle, so that the total change in $\arg f(s)$ equals the total change in $\arg f(-s)$, and since their sum is the total change in $\arg f(s)f(-s) = \arg A$, i.e., zero, the total change in $\arg f(s)$ is also 0. Thus the definition (3.3) makes sense; it is only necessary to specify the

additive multiple of $2\pi i$ and we do this in such a way that

$$\Phi(s) \sim \pm \alpha s + o(s), \qquad |R l s| \to \infty, \qquad (3.4)$$

in conformity with the asymptotic condition (2.7).

Putting (3.3) into (3.2), and using (2.7), the boundary condition on the cut takes the form

$$\Phi^+(t) = \Phi^-(t) = \ln A + 2\pi m i, \qquad (3.5)$$

where m is some integer.

Boundary-value problems of this form are discussed[3] in Sec. 84 of M. Since $f(s)$ is bounded in any finite region of the cut plane and on its boundaries [by (2.3)] and is therefore also bounded away from zero [by (2.4′)], its logarithm $\Phi(s)$ is bounded. Thus the solutions of (3.4) we are interested in are those which, in the terminology defined on p. 231 of M, belong to the class h $(-2\mu, 2\mu)$ (i.e., they are bounded at both ends of the cut.)

A particular solution of the boundary-value problem satisfying this condition is the function

$$\tfrac{1}{2}(\ln A + 2\pi m i).$$

The general solution of (3.5) is obtained from this particular solution by adding the general solution of the associated homogeneous equation $\Phi^+(t) + \Phi^-(t) = 0$. According to the theory described in Secs. 35 and 79 of M, this general solution, of finite degree at infinity, is of the form

$$X(s)P(s),$$

where P is a polynomial and X is the "fundamental solution" of the homogeneous problem. This fundamental solution is (see p. M232) the one which is nowhere zero in the finite part of the plane, including the cut, except at the two end points -2μ and 2μ. The appropriate solution, given in Eq. (84.3) of M, is $\sqrt{E(s)}$, and so we have for our general solution

$$\Phi(s) = \tfrac{1}{2}(\ln A + 2\pi m i) + \sqrt{E(s)}P(s), \qquad (3.6)$$

where $P(s)$ is a polynomial. The condition (3.4) determines this polynomial as $P(s) = \pm \alpha$, and, putting the resulting formula for $\Phi(s)$ into (3.3), we obtain

$$f(s) = \pm \sqrt{A} \exp[\pm \alpha \sqrt{E(s)}], \qquad (3.7)$$

a formula in which there are two choices of sign.

The solution of the original functional equation for the one-dimensional case is therefore, by (2.3),

$$\psi(s) = \pm \sqrt{A} \cosh\alpha\sqrt{E(s)}, \qquad (3.8)$$

$$\phi(s) = \pm \sqrt{A}[\sinh\alpha\sqrt{E(s)}]/\sqrt{E(s)}, \qquad (3.9)$$

again with two choices of sign. This is the solution given in Eqs. (3.58) and (3.59) of LZ.

4. THE THREE-DIMENSIONAL CASE

To deal with this case, we return to the general form of the boundary-value problem given in (2.10). Now $E(s)$ is a polynomial of degree 6. We denote its roots

by $\pm s_1, \pm s_2, \pm s_3$, with s_2 and $s_3 - s_1$ real, and choose the cuts as shown in Fig. 1.

Another new feature is that now $V(t)$ is a polynomial of degree 8, so that $f(s)$ and $f(-s)$ must have zeros in the cut plane or on its boundaries. In fact, if the zeros of $f(s)$ are z_1, z_2, z_3, z_4, then those of $f(-s)$ are $-z_1, -z_2, -z_3, -z_4$ and so those of $V(s)$ are $\pm z_1, \pm z_2, \pm z_3, \pm z_4$. We assume that $V(s)$ and $E(s)$ have no zeros in common, so that none of $\pm z_1, \ldots, \pm z_4$ is the end of a cut. Let us define

$$F(s) = f(s) \prod_{i=1}^{4} (s - z_i)^{-1} \qquad (4.1)$$

so that, by (2.10),

$$F(s)F(-s) = V(s) \prod_{i=1}^{4} [(s - z_i)(s + z_i)]^{-1} = c, \qquad (4.2)$$

where c is the coefficient of s^8 in $V(s)$ (it is $-a_1 h_1$ in the notation of LZ). Thus F satisfies a functional equation like the one we solved before. The boundary conditions are

$$|F(s)| = \exp[\pm \alpha R l s + o(s)] \qquad (4.3)$$

for large $|(R l s)|$, and

$$F^+(t)F^-(t) = cJ(t) \qquad (t \in C), \qquad (4.4)$$

where

$$J(t) = V(t)[c \prod_{i=1}^{4} (t - z_i)]^{-2} = \prod_{i=1}^{4} \frac{(t + z_i)}{(t - z_i)} \qquad (4.5)$$

and C denotes the set of cuts.

Since there are now three cuts, it is not as easy as before to define a function Φ to serve as $\ln F$. By considering the behavior of $F(s)$ as s traverses a large circle, we can show that $\arg F(s)$ returns to its original value if s traverses a contour that encircles all three cuts, and, by considering a symmetrical contour that encloses only the cut through the origin, we can show that $\arg F(s)$ returns to its original value as s
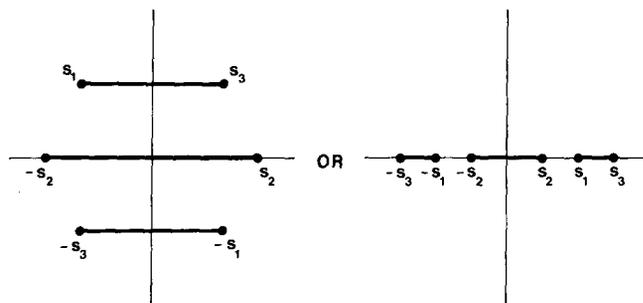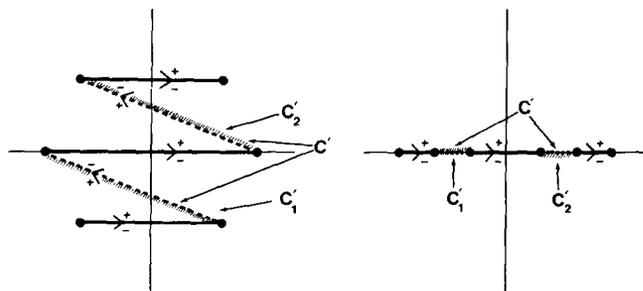

FIG. 1. Cuts C in the s plane.

FIG. 2. Cuts C' in the s plane.

traverses any contour enclosing only this cut; but there is as yet no reason to expect $\arg F(s)$ to return to its original value if s traverses a contour that surrounds one of the other cuts. To deal with this, we put two further cuts C' as shown dotted in Fig. 2.

We can now define a function

$$\Phi(s) = \ln F(s), \tag{4.6}$$

which is holomorphic in the cut plane and satisfies

$$\Phi^+(t) + \Phi^-(t) = \ln c + 2\pi m i + \ln J(t) \quad (t \in C),$$
$$\Phi^+(t) - \Phi^-(t) = 2\pi n i \quad (t \in C'), \tag{4.7}$$

where m and n are integers. The reason why we can use the same value of n on both parts of C' is that we know [since $F(s)F(-s) = c$] that if s traverses a symmetrical path enclosing only the part of C containing the origin, then $\arg F$ will return to its original value and so the discontinuities of Φ across the two parts of C' must be the same.

Equation (4.7) is again a Hilbert problem, of the type discussed in Secs. 85–87 of M. As before, its general solution is the sum of a particular solution and the general solution of the associated homogeneous problem. For a particular solution, consider the function [obtained from Eq. M (85.12)]

$$\Phi(s) = \tfrac{1}{2}\ln c + \pi m i + \frac{\sqrt{E(s)}}{2\pi i} \int_C \frac{\ln J(t) dt}{\sqrt{E^+(t)}(t-s)}$$
$$+ \frac{\sqrt{E(s)}}{2\pi i} \int_{C'} \frac{2\pi n i \, dt}{\sqrt{E^+(t)}(t-s)}, \tag{4.8}$$

where the cuts are traversed in the directions indicated in Fig. 2, and their "plus" sides are at the left of the arrows. The Plemelj formulas (p. M43) show that this is a particular solution of the boundary-value problem (4.7). To get the general solution, we add $X(s)P(s)$ where P is any polynomial and X is the fundamental solution of the class we are looking for. As before, since we want bounded solutions, this fundamental solution is $\sqrt{E(s)}$. Our asymptotic condition (4.3) implies, however, that the polynomial P must be 0, since $\sqrt{E(s)}$ increases like s^3, not s, for large $|(R/s)|$. Thus the particular solution (4.8) itself is the one we are looking for.

To get the correct behavior for large s, we want

$$\Phi(s) \sim \pm \alpha s \quad \text{for large } s,$$

and, since $E(s) \sim s^3$, this implies that the sum of the two integrals must behave like $\pm 2\pi i \alpha / s^2$ for large s. The asympototic behavior of these integrals is obtained from the formula $(t-s)^{-1} = -s^{-1} - ts^{-2}\cdots$, and

so we require [writing $\sqrt{E}(t)$ as an abbreviation for $^s\sqrt{E^+(t)}$]

$$\frac{1}{2\pi i} \int_C \frac{\ln J(t) dt}{\sqrt{E}(t)} + n \int_{C'} \frac{dt}{\sqrt{E}(t)} = 0 \tag{4.9}$$

(coefficient of s^{-1}), and

$$\frac{1}{2\pi i} \int_C \frac{t \ln J(t) dt}{\sqrt{E}(t)} + n \int_{C'} \frac{t dt}{\sqrt{E}(t)} = \mp \alpha \tag{4.10}$$

(coefficient of s^{-2}).

Now, Eq. (4.5) shows that $\ln J(t)$ is an odd function; hence, the first integral in (4.9) is zero. The second can be written

$$\int_{C_1'} \frac{dt}{\sqrt{E^+(t)}} - \int_{C_2'} \frac{dt}{\sqrt{E^-(t)}}. \tag{4.11}$$

The sides of the contours on which the integrand is evaluated are indicated in Fig. 2, and are symmetrical. Since $\sqrt{E}(s)$ is an odd function, it follows that the two integrals reinforce and so [barring the accident $\int dt/\sqrt{E}(t) = 0$] the condition (4.9) can only be satisfied by taking $n = 0$. The second condition, (4.10), now reduces to

$$\alpha = \mp \frac{1}{2\pi i} \int_C \frac{t \ln J(t) dt}{\sqrt{E}(t)}, \tag{4.12}$$

which imposes a condition on the coefficients $h_i, \ldots, a_4$ in the polynomials $E(s)$ and $V(s)$.

The solution of the functional equation for f is, by (4.6) and (4.1),

$$f(s) = \pm \sqrt{c} \prod_{i=1}^{4} (s - z_i) \left\{ \exp \frac{\sqrt{E(s)}}{2\pi i} \int_C \frac{\ln J(t) dt}{\sqrt{E^+(t)}(t-s)} \right\} \tag{4.13}$$

There are several solutions, depending upon the choice of the sign in (4.13) and which four zeros of V we pick to use as $z_1, \ldots, z_4$. We expect that, as in the one-dimensional case, physical requirements will dictate a unique choice. This will certainly be true at low densities where the PY solution can be found from a convergent virial expansion.[4] At higher densities we expect to see a phase transition corresponding to a spatial separation of the two components since α in (1.2) is positive. We plan to investigate this further.

ACKNOWLEDGMENT

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