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ON THE TWO-SPHERE PROBLEM IN AN ABSORBING MEDIUM

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Работа посвящена решению абсорбционной задачи двух сфер, которая состоит в следующем. В неограниченной матрице содержатся две непересекающиеся сферы одинакового радиуса, в которых генерируются дефекты с постоянной скоростью. Дефекты поглощаются матрицей и сферами с различными коэффициентами абсорбции. Требуется определить стационарное распределение дефектов в среде. Эта задача возникает естественным образом при вычислении эффективного коэффициента абсорбции случайной суспенсии сфер. Предложенное аналитическое решение использует т. наз. метод двойных разложений, который удобен для численной реализации.

Mikhail Kolev. ON THE TWO-SPHERE PROBLEM IN AN ABSORBING MEDIUM

The paper is devoted to the two-sphere absorption problem. Namely, let two identical spheres be embedded into an unbounded matrix. Defects are created within the spheres at constant rate and are absorbed, with different absorption coefficients, by the matrix and the spheres. The steady-state defect distribution in the medium has to be found. This problem appears in a natural way when evaluating the effective absorption coefficient of a random dispersion of spheres. The herein proposed analytical solution employs the twin-expansions method and it is convenient for numerical implementation.

1. INTRODUCTION

Consider the equation

$$\Delta H^{(2)}(\mathbf{x};\mathbf{z}) - \left\{k_m^2 + [k^2]\big(h(\mathbf{x}) + h(\mathbf{x}-\mathbf{z})\big)\right\} H^{(2)}(\mathbf{x};\mathbf{z}) - [k^2]\left\{h(\mathbf{x}) + h(\mathbf{x}-\mathbf{z})\right\} = 0. \tag{1}$$

Here $h(\mathbf{x})$ is the characteristic function of a sphere of radius a located at the origin, $[k^2] = k_f^2 - k_m^2$; the differentiation everywhere is with respect to $\mathbf{x}$, $\mathbf{z}$ plays the role of a parameter, $|\mathbf{z}| > 2a$. The solution $H^{(2)}(\mathbf{x};\mathbf{z})$, we are seeking, should be bounded and continuous everywhere in $\mathbb{R}^3$, and its normal derivative should be continuous on the surfaces $|\mathbf{x}| = a$ and $|\mathbf{z}-\mathbf{x}| = a$. The interpretation of eqn (1) is as follows. It describes the steady-state distribution $H^{(2)}(\mathbf{x};\mathbf{z})$ of a diffusing species (say, irradiation defects) generated within two non-overlapping spheres, embedded into an unbounded matrix, at the rate $-[k^2]$. The spheres are of radius a, located at the origin and at the point $\mathbf{z}$. The species is then absorbed by the spheres and by the matrix with different (and positive) absorption coefficients k_f^2 and k_m^2 respectively. Due to this interpretation, the problem (1) was called in [1,2] the two-sphere absorption problem. Let us recall that this problem appeared in a natural way in [1,2] when looking for the effective absorption coefficient of a random dispersion of spheres to the order c^2, where c is the volume fraction of the spheres. Hence, the solution of (1), especially in a form suitable for numerical implementation, is needed when evaluating the statistical characteristics of the diffusing species field in the random dispersion and, in particular, when calculating the effective absorption coefficient of the latter. The aim of this paper to describe such a solution of the problem (1), using the method of twin-expansions. It is to be pointed out that a similar method has been successfully employed in the respective two-spheres problems for heat conduction [3,4], elasticity [5], diffraction [6], etc.

2. TWIN-EXPANSION SOLUTION OF THE PROBLEM (1)

Let us introduce two Cartesian systems and two systems of spherical co-ordinates as shown in Fig. 1. Both spheres are of radius a, the origins of the systems are at the centres of the spheres, the χ-co-ordinate is common for them, and the distance between the centres, $|O_1O_2|$, is denoted by R, so that

$$x_1 = x_2, \quad y_1 = y_2, \quad z_1 = z_2 + R.$$

Then, obviously,

$$x_1 = r_1 \sin\theta_1 \cos\chi, \quad x_2 = r_2 \sin\theta_2 \cos\chi,$$

$$y_1 = r_1 \sin\theta_1 \sin\chi, \quad y_2 = r_2 \sin\theta_2 \sin\chi,$$

$$z_1 = r_1 \cos\theta_1, \qquad z_2 = -r_2 \cos\theta_2,$$

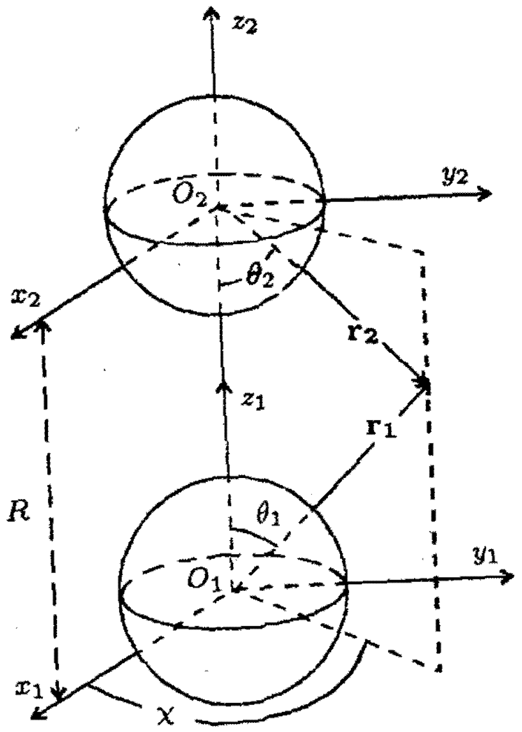

Fig. 1

where $0 \leqq r_1, r_2 < \infty$, $0 \leqq \theta_1, \theta_2 \leqq \pi$, $0 \leqq \chi < 2\pi$.

We need, first of all, a convenient form of the relation between the spherical wave functions given in the two spherical co-ordinate systems. We start with the identity [6]:

$$(2) \qquad Z_n^{(1)}(k_m r_2) P_n(\cos\theta_2) = (-1)^n \sum_{s=0}^{\infty} Q_{oson}(k_m R, \pi) j_s(k_m r_1) P_s(\cos\theta_1),$$

where

$$(3) \qquad Z_n^{(1)}(k_m r_2) = \sqrt{\frac{\pi}{2k_m r_2}} H^{(1)}_{n+\frac{1}{2}}(k_m r_2), \quad j_s(k_m r_1) = \sqrt{\frac{\pi}{2k_m r_1}} J_{s+\frac{1}{2}}(k_m r_1)$$

are the spherical Bessel functions,

$$H_n^{(1)}(z) = J_m(z) + iN_m(z)$$

denotes as usual the Hankel function of the first kind,

$$(4) \quad Q_{oson}(k_m R, \pi) = \frac{2i^{s-n}}{N_{os}} \sum_{\sigma=|s-n|}^{s+n} i^\sigma b_\sigma^{(sono)} Z_\sigma^{(1)}(k_m R) P_\sigma(-1), \quad N_{os} = \frac{2}{2s+1},$$

$P_s(x)$ are the Legendre polynomials, and

$$b_n^{(n_1 m_1 n_2 m_2)} = (-1)^{m_2} \sqrt{\frac{(n_1+m_1)!(n_2+m_2)!(n-m_1+m_2)!}{(n_1-m_1)!(n_2-m_2)!(n+m_1-m_2)!}}$$

$$\times\, (n_1 n_2 oo|no)(n_1 n_2 m_1, -m_2|n, m_1 - m_2),$$

where $(n_1 n_2 m_1 m_2 | n, m_1 + m_2)$ are the Clebsh–Gordan coefficients.

According to the fact that $P_\sigma(-1) = (-1)^\sigma$, we have from (2):

$$\sqrt{\frac{\pi}{2k_m r_2}} H^{(1)}_{n+\frac{1}{2}}(k_m r_2) P_n(\cos\theta_2) = (-1)^n \sqrt{\frac{\pi}{2k_m r_1}} \sqrt{\frac{\pi}{2k_m R}} \sum_{s=0}^{\infty} J_{s+\frac{1}{2}}(k_m r_1) \tag{5}$$

$$\times P_s(\cos\theta_1) \frac{2i^{s-n}}{N_{0s}} \sum_{\sigma=|s-n|}^{s+n} (-i)^\sigma b_\sigma^{(s0n0)} H^{(1)}_{\sigma+\frac{1}{2}}(k_m R).$$

Using the well-known relations between the Bessel functions:

$$I_{s+\frac{1}{2}}(x) = i^{-(s+\frac{1}{2})} J_{s+\frac{1}{2}}(ix), \quad K_{s+\frac{1}{2}}(x) = \frac{\pi i}{2} i^{(s+\frac{1}{2})} H^{(1)}_{s+\frac{1}{2}}(ix), \tag{6}$$

we find from (5) the formula

$$\frac{1}{\sqrt{k_m r_2}} K_{n+\frac{1}{2}}(k_m r_2) P_n(\cos\theta_2) = (-1)^n \sqrt{\frac{2\pi}{k_m R}} \frac{1}{\sqrt{k_m r_1}} \tag{7}$$

$$\times \sum_{s=0}^{\infty} \frac{(-1)^s}{N_{os}} I_{s+\frac{1}{2}}(k_m r_1) P_s(\cos\theta_1) \Big[\sum_{\sigma=|s-n|}^{s+n} (-1)^\sigma b_\sigma^{(sono)} K_{\sigma+\frac{1}{2}}(k_m R) \Big]$$

between the spherical wave functions in the two co-ordinate systems (Fig. 1), which is just the form suitable for our purposes.

We look for the solution $H^{(2)}(\mathbf{x};\mathbf{z})$ of the eqn (1), that is independent of the co-ordinate φ, in the following form:

— inside the sphere "i" as

$$H^{(2)}_{(i)} = -\frac{[k^2]}{k_f^2} + \sum_{n=0}^{\infty} A_n \sqrt{\frac{a}{r_i}} I_{n+\frac{1}{2}}(k_f r_i) P_n(\cos\theta_i), \quad i = 1, 2; \tag{8a}$$

— outside the spheres as

$$H^{(2)}_{(out)} = \sum_{n=0}^{\infty} \Big\{ C_n^{(1)} \sqrt{\frac{a}{r_1}} K_{n+\frac{1}{2}}(k_m r_1) P_n(\cos\theta_1) \tag{8b}$$

$$+ C_n^{(2)} \sqrt{\frac{a}{r_2}} K_{n+\frac{1}{2}}(k_m r_2) P_n(\cos\theta_2) \Big\}.$$

Due to the obvious symmetry of the problem under study we have $C_n = C_n^{(1)} = C_n^{(2)}$, $n = 0, 1, \ldots$ Thus

$$H^{(2)}_{(out)} = \sum_{n=0}^{\infty} C_n \Big\{ \sqrt{\frac{a}{r_1}} K_{n+\frac{1}{2}}(k_m r_1) P_n(\cos\theta_1) \tag{9}$$

$$+ \sqrt{\frac{a}{r_2}} K_{n+\frac{1}{2}}(k_m r_2) P_n(\cos\theta_2) \Big\}.$$

The coefficients A_n and C_n are to be found from the above mentioned boundary conditions, namely, the continuity of the field $H^{(2)}(\mathbf{x};\mathbf{z})$ and its normal derivative across each spherical interface (with respect to $\mathbf{x}$; recall that $\mathbf{z}$ plays the role of a parameter).

According to (7), we recast the solution (8b) of eqn (1) outside the spheres as

$$H^{(2)}_{(out)} = \sqrt{\frac{a}{r_1}} \sum_{n=0}^{\infty} P_n(\cos\theta_1)\Big\{C_n K_{n+\frac{1}{2}}(k_m r_1) + \sqrt{\frac{2\pi}{k_m R}} \frac{1}{N_{on}} I_{n+\frac{1}{2}}(k_m r_1)$$

(10)

$$\times \sum_{s=0}^{\infty} (-1)^{n+s} C_s \Big[\sum_{\sigma=|s-n|}^{s+n} (-1)^{\sigma} b_{\sigma}^{(sono)} K_{\sigma+\frac{1}{2}}(k_m R)\Big]\Big\}.$$

Making use of the above mentioned boundary conditions, the orthogonality of the Legendre polynomials and the fact that $b^{(sooo)} = 1$, $s = 0, 1, \ldots$, see [6], we find the following relations between the unknown coefficients

(11a) $$A_0 I_{\frac{1}{2}}(a_f) - \frac{[k^2]}{k_f^2} = C_0 K_{\frac{1}{2}}(a_m) + \frac{1}{N_{oo}} I_{\frac{1}{2}}(a_m) \sqrt{\frac{2\pi}{k_m R}} \left[\sum_{s=0}^{\infty} C_s K_{s+\frac{1}{2}}(k_m R)\right],$$

$$A_n I_{n+\frac{1}{2}}(a_f) = C_n K_{n+\frac{1}{2}}(a_m) + \frac{1}{N_{on}} I_{n+\frac{1}{2}}(a_m) \sqrt{\frac{2\pi}{k_m R}}$$

(11b)

$$\times \left[\sum_{s=0}^{\infty} C_s \Big(\sum_{\sigma=|s-n|}^{s+n} (-1)^{n+s+\sigma} b_{\sigma}^{(sono)} K_{\sigma+\frac{1}{2}}(k_m R)\Big)\right], \quad n = 1, 2, \ldots,$$

$$A_0[2a_f I'_{\frac{1}{2}}(a_f) - I_{\frac{1}{2}}(a_f)] = C_0 \left[2a_m K'_{\frac{1}{2}}(a_m) - K_{\frac{1}{2}}(a_m)\right]$$

(12a)

$$+ \frac{1}{N_{oo}} \sqrt{\frac{2\pi}{k_m R}} [2a_m I'_{\frac{1}{2}}(a_m) - I_{\frac{1}{2}}(a_m)] \sum_{s=0}^{\infty} C_s K_{s+\frac{1}{2}}(k_m R),$$

$$A_n[2a_f I'_{n+\frac{1}{2}}(a_f) - I_{n+\frac{1}{2}}(a_f)] = C_n \left[2a_m K'_{n+\frac{1}{2}}(a_m) - K_{n+\frac{1}{2}}(a_m)\right]$$

(12b) $$+ \frac{1}{N_{on}} \sqrt{\frac{2\pi}{k_m R}} \left[2a_m I'_{n+\frac{1}{2}}(a_m) - I_{n+\frac{1}{2}}(a_m)\right]$$

$$\times \left[\sum_{s=0}^{\infty} C_s \Big(\sum_{\sigma=|s-n|}^{s+n} (-1)^{n+s+\sigma} b_{\sigma}^{(sono)} K_{\sigma+\frac{1}{2}}(k_m R)\Big)\right], \quad n = 1, 2, \ldots$$

Simple manipulations, employing the well-known properties

$$I'_s(x) = \frac{1}{2}[I_{s+1}(x) + I_{s-1}(x)], \quad K'_s(x) = -\frac{1}{2}[K_{s+1}(x) + K_{s-1}(x)]$$

of the modified Bessel functions, allow to exclude A_n from eqns (11), so that (12) yields the needed equations for the coefficients C_n:

$$
\begin{aligned}
&C_0 U_0 + V_0 \sum_{s=0}^{\infty} C_s K_{s+\frac{1}{2}}(k_m R) = -2\frac{[k^2]}{k_f^2} a_f I_{\frac{3}{2}}(a_f), \\
(13)\qquad & \\
&C_n U_n + V_n \sum_{s=0}^{\infty} C_s \left[\sum_{\sigma=|s-n|}^{s+n} (-1)^{n+s+\sigma} b_\sigma^{(sono)} K_{\sigma+\frac{1}{2}}(k_m R) \right] = 0,
\end{aligned}
$$

$n = 1, 2, \ldots$, where

$$
\begin{aligned}
U_n &= a_f K_{n+\frac{1}{2}}(a_m)\left[I_{n-\frac{1}{2}}(a_f) + I_{n+\frac{3}{2}}(a_f)\right] \\
&\quad + a_m I_{n+\frac{1}{2}}(a_f)\left[K_{n-\frac{1}{2}}(a_m) + K_{n+\frac{3}{2}}(a_m)\right],
\end{aligned}
\tag{14a}
$$

$$
\begin{aligned}
V_n &= \frac{1}{N_{on}}\sqrt{\frac{2\pi}{k_m R}}\Big\{a_f I_{n+\frac{1}{2}}(a_m)\left[I_{n-\frac{1}{2}}(a_f) + I_{n+\frac{3}{2}}(a_f)\right] \\
&\quad - a_m I_{n+\frac{1}{2}}(a_f)\left[I_{n-\frac{1}{2}}(a_m) + I_{n+\frac{3}{2}}(a_m)\right]\Big\},
\end{aligned}
\tag{14b}
$$

and $a_f = ak_f$, $a_m = ak_m$ are dimensionless parameters.

For the coefficients A_n we get in turn:

$$
A_0 = \frac{1}{I_{\frac{1}{2}}(a_f)}\left\{\frac{[k^2]}{k_f^2} + C_0 K_{\frac{1}{2}}(a_m) + \frac{1}{2} I_{\frac{1}{2}}(a_m)\sqrt{\frac{2\pi}{k_m R}} \sum_{s=0}^{\infty} C_s K_{s+\frac{1}{2}}(k_m R)\right\},
\tag{15a}
$$

$$
\begin{aligned}
A_n &= \frac{1}{I_{n+\frac{1}{2}}(a_f)}\Big\{C_n K_{n+\frac{1}{2}}(a_m) + \frac{1}{N_{on}} I_{n+\frac{1}{2}}(a_m)\sqrt{\frac{2\pi}{k_m R}} \\
&\quad \times \Big[\sum_{s=0}^{\infty} C_s \Big(\sum_{\sigma=|s-n|}^{s+n} (-1)^{n+s+\sigma} b_\sigma^{(sono)} K_{\sigma+\frac{1}{2}}(k_m R)\Big)\Big]\Big\}, \quad n = 1, 2, \ldots
\end{aligned}
\tag{15b}
$$

In this way the two-sphere problem (1) is reduced to the solution of the infinite system of linear equations (13) for any given separation distance R between the spheres.

The natural numerical procedure to solve the problem (1) is the method of truncation. Namely, assuming $C_n = 0$ at $n > N$ in (13), we get a linear system of $N+1$ equations for the first $N+1$ coefficients C_n, $n = 0, 1, \ldots$ Solving the latter, we find the approximate values $C_n^{(N)}$ of these coefficients. Then, at $N \to \infty$, the approximations $C_n^{(N)}$ will converge to the exact values C_n, as we shall argue in the next section.

Due to the exponential decay of the modified Bessel functions $K_{n+\frac{1}{2}}(x)$, $n = 0, 1, \ldots$ the series solution developed in the present section converges very rapidly when the spheres are well apart. For instance, to obtain the values of the coefficients A_n, C_n and the field $H^{(2)}(\mathbf{x};\mathbf{z})$ with three decimal digits, it suffices to take $N = 10$ if $R/a \geqq 3$. However, as the spheres approach each other, more equations should be kept in the truncated system, e.g. at $2.1 < a/R < 3$ we should take $N = 20$ in order to have the same three decimal digits correct.

3. JUSTIFICATION OF THE TRUNCATION METHOD

To justify the above used truncation method a bit more detailed investigation of the infinite system (13) is needed. With this aim in view we recast it in the form

(16)
$$C_0 + \frac{U_0}{V_0}\sum_{s=0}^{\infty} C_s K_{s+\frac{1}{2}}(k_m R) = -2\frac{[k^2]}{k_f^2}\frac{a_f I_{\frac{3}{2}}(a_f)}{U_0},$$
$$C_n + \frac{V_n}{U_n}\sum_{s=0}^{\infty} C_s\left[\sum_{\sigma=|s-n|}^{s+n}(-1)^{n+s+\sigma} b_\sigma^{(sono)} K_{\sigma+\frac{1}{2}}(k_m R)\right] = 0,$$

$n = 1, 2, \dots$ In turn, using the relations (6) and the definition (4) of Q_{oson}, we rewrite eqn (16) as

(17)
$$C_n + \sum_{s=0}^{\infty} d_{sn} C_s = f_n, \quad n = 0, 1, \dots$$

where

(18a)
$$d_{sn} = \frac{\pi}{2} i^{3s+n+2} Q_{onos}(ik_m R, \pi)\frac{W_n}{U_n}, \quad s, n = 0, 1, \dots$$

(18b)
$$f_n = \begin{cases} -2\frac{[k^2]}{k_f^2}\frac{a_f I_{\frac{3}{2}}(a_f)}{U_0}, & \text{if } n = 0, \\ 0, & \text{otherwise,} \end{cases}$$

(18c)
$$W_n = N_{on}\sqrt{\frac{k_m R}{2}}V_n.$$

Let us replace in the system (17) the unknowns C_n by X_n:

(19)
$$C_n = I_{n+\frac{1}{2}}(a_m)X_n.$$

The infinite set of equations (17), when written with respect to the new unknowns X_n, becomes

(20)
$$X_n + \sum_{s=0}^{\infty} D_{sn} X_s = g_n, \quad n = 0, 1, \dots$$

where

(21)
$$D_{sn} = d_{sn}\frac{I_{s+\frac{1}{2}}(a_m)}{I_{n+\frac{1}{2}}(a_m)}, \quad g_n = \frac{f_n}{I_{n+\frac{1}{2}}(a_m)}.$$

The asymptotical behaviour of the coefficients D_{sn}, for large values of s, n, can be easily deduced by means of the Debay formulae [7, p. 25]:

(22)
$$K_\lambda(x) \sim \sqrt{\frac{\pi}{2\lambda}}\left(\frac{2\lambda}{ex}\right)^\lambda, \quad I_\lambda(x) \sim \frac{1}{\sqrt{2\pi\lambda}}\left(\frac{2\lambda}{ex}\right)^{-\lambda} \quad \text{for } \lambda \gg x.$$

Introducing (22) into the definitions (14a) and (18c) of the coefficients U_n and W_n we find, after simple algebra, that

(23)
$$\left|\frac{W_n}{U_n}\right| < c_1(2n+3)\left(\frac{ea_m}{2n+1}\right)^{2n+1}, \quad n = 0, 1, \ldots$$

with a certain constant c_1.

For bounding the function Q_{onos} we use the result of Ivanov [6]:

(24)
$$|Q_{onos}| < \frac{c_2 s(2s+2n+1)^{n+s}}{(k_m R)^{3/2}(ek_m R)^{n+s+\frac{1}{2}}},$$

where c_2 is another constant.

We next introduce (22), (23) and (24) into (21) and take into account (18a):

(25)
$$|D_{sn}| < c\frac{s}{2s+1}\left(\frac{2n+2s+1}{2n+1}\right)^n\left(\frac{2n+2s+1}{2s+1}\right)^s\left(\frac{a}{R}\right)^{n+s+1},$$

$s, n = 0, 1, \ldots$

Since $R > 2a$ (the spheres are nonoverlapping), $a/R < \frac{1}{2}$ and thus

(26a)
$$\sum_{s,n=0}^{\infty} |D_{sn}|^2 < \infty.$$

Let us note that obviously

(26b)
$$\sum_{n=0}^{\infty} |g_n|^2 < \infty.$$

Hence the system (20) can be recast as

(27)
$$\mathbf{X} + \mathbf{D}\cdot\mathbf{X} = \mathbf{G},$$

where $\mathbf{X} = \{X_n\}$, $\mathbf{G} = \{g_n\}$ and $\mathbf{D} = \{D_{sn}\}$, $s, n = 0, 1, \ldots$, Due to (26), eqn (27) is an equation in the Hilbert space ℓ^2 with a compact operator $\mathbf{D}$, so that the Fredholm alternative holds [8, Ch. 13]. Therefore, in particular, the system (27) will have a unique solution for any $\mathbf{G} \in \ell^2$ if the homogeneous system (27) possesses a unique (trivial) solution. But the latter is obviously the case for our problem, since $\mathbf{G} = \mathbf{0}$ corresponds to $[k^2] = 0$, i.e. to a homogeneous equation (1). (The homogeneous equation (1) has a trivial solution only, since the absorption coefficients k_f^2 and k_m^2 are positive.) The uniqueness and existence theorem for infinite system (13) is thus proved. Its obvious corollary is then the needed justification of the truncation method of Section 2: due to (26a), the solutions $C_n^{(N)}$ of the truncated systems (13) will indeed converge in ℓ^2 to the solution of (13) at $N \to \infty$.

4. CONCLUDING REMARKS

In this note we have presented and justified a method of effective numerical solution of the two-sphere problem (1). When combined with the general results of [2], concerning diffusion of defects in a random dispersion, it allows to obtain, in particular, the effective absorption coefficient k^{*2} of the dispersion and the two-point correlation function of the defect fields to the order c^2. More details and the respective numerical results are given in [2].

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