The Solution of the Modified Helmholtz Equation in a Triangular Domain and an Application to Diffusion-Limited Coalescence

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A new transform method for solving boundary value problems for linear and integrable nonlinear PDEs recently introduced in the literature is used here to obtain the solution of the modified Helmholz equation $q_x(x,y) + q_y(x,y) - 4\beta^2 q(x,y) = 0$ in the triangular domain $0 \leq x \leq L - y \leq L$, with mixed boundary conditions. This solution is applied to the problem of diffusion-limited coalescence, $A + A \rightleftharpoons A$, in the segment $(-L/2, L/2)$, with traps at the edges.

\textit{I. INTRODUCTION}

A new method for solving boundary value problems for linear and for integrable nonlinear PDEs has been introduced recently \cite{1}. Here we apply this method to the equation

$$E_{xx} + E_{yy} + \gamma(-E_x + E_y) = 0 ,$$

in the triangular domain $-L/2 \leq x \leq y \leq L/2$, where $E(x,y)$ is a scalar function and $\gamma$ is a positive constant. A solution of Eq. (1.1) in the semi-infinite wedge $0 \leq x \leq y$ has been presented in \cite{2}. Using the substitution $E(x,y) = 1 - e^{-2/(y-x)}q(x,y)$, Eq. (1.1) becomes the modified Helmholz equation

$$q_{xx} + q_{yy} - 4\beta^2 q = 0 , \quad \beta = \frac{\gamma}{\sqrt{8}} .$$

Eq. (1.1) with $\gamma = v/D$ represents the steady state of the diffusion-limited reaction $A + A \rightleftharpoons A$ on the line, where the $A$-particles diffuse with diffusion constant $D$, they merge immediately upon encounter, and split into two particles (the back reaction) at rate $v$. $E(x,y)$ represents the probability that the interval $(x,y)$ is empty. The concentration profile of the particles is related to $E(x,y)$ through $c(x) = -E_y(x,y)$. Suppose that we limit ourselves to the segment $-L/2 \leq x \leq y \leq L/2$, then the domain of Eq. (1.1) is $-L/2 \leq x \leq y \leq L/2$. The forward reaction is described by the boundary condition (BC) $E(x,x) = 1$. If there are perfect traps at the edges, $x = \pm L/2$, one gets the BCs $E_x(-L/2,y) = 0, E_y(x,L/2) = 0$. These BCs transform into the following BCs for Eq. (1.2):

$$q(x,x) = 0 , \quad -\frac{L}{2} \leq x \leq \frac{L}{2} ,$$

$$\frac{\gamma}{2} q(-\frac{L}{2}, y) + q_x(-\frac{L}{2}, y) = 0 , \quad -\frac{L}{2} \leq y \leq \frac{L}{2} ,$$

$$-\frac{\gamma}{2} q(x, \frac{L}{2}) + q_x(x, \frac{L}{2}) = 0 , \quad -\frac{L}{2} \leq x \leq \frac{L}{2} .$$

We rotate and translate the $(x,y)$-axes, with the mapping $(x,y) \mapsto (-y + L/2, x + L/2)$. Eq. (1.2) remains invariant, but the domain is now $0 \leq x \leq L - y \leq L$ — the isosceles right triangle with vertices at $(0,0)$, $(0,L)$, $(L,0)$ — and the BCs become

$$q(x,L-x) = 0 , \quad 0 \leq x \leq L , \quad (1.3a)$$

$$\frac{\gamma}{2} q(x,0) + q_y(x,0) = 0 , \quad 0 \leq x \leq L , \quad (1.3b)$$

$$\frac{\gamma}{2} q(0,y) + q_x(0,y) = 0 , \quad 0 \leq y \leq L . \quad (1.3c)$$

For the sake of generality, instead of the BC (1.3b), (1.3c) we consider

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where \( f(\cdot) \) is an arbitrary smooth function.

We will show that: (a) Eq. (1.2) with the BCs (1.3a), (1.3b), (1.3c) has a unique solution that can be expressed in closed form. (b) Eq. (1.2) with the homogeneous BCs (1.3a), (1.3b), (1.3c) has only the trivial solution \( q(x,y) = 0 \). i.e., the only steady state of the process \( A + A \not\rightarrow A \), in a segment demarcated by traps, is the vacuum — when there are no particles left — regardless of the magnitude of \( v \).

Indeed, for the derivation of (2.3a) we use \( z = x \), and we note that the boundary condition (1.3b) implies

\[
\frac{1}{2}(q_x(x,0) - i q_y(x,0)) + \frac{\alpha^2}{k} q(x,0) = \frac{1}{2} q_x(x,0) + i(\frac{\alpha^2}{k} + \frac{\pi}{4}) q(x,0) - \frac{i}{2} f(x)
\]

integrating by parts the terms involving \( q_x \) we find (2.3a). The derivation of (2.3b) is similar, where we use the condition (1.3c). For the derivation of (2.3c) we use \( z = i L + x - i x \), and we note that the boundary condition \( q(x,L - x) = 0 \) implies \( q_x(x,L - x) - q_y(x,L - x) = 0 \).

In order to simplify the analysis, we have assumed that the same function \( f \) appears in the BCs (1.3b) and (1.3c). This implies that the PDE (1.2), the triangular domain, and the BCs (1.3a), (1.3b''), (1.3c) are invariant under the reflection \( x \leftrightarrow y \), thus \( q(x,y) = q(y,x) \). Hence, \( \psi_1(k) = \psi_2(k) \).

We introduce the following notations:

\[
\psi_1(k) = \psi_2(k) = \varphi(k), \quad \psi_3(-ke^{-i\pi/4}) = \psi(-), \quad \psi_3(-ke^{i\pi/4}) = \psi(+), \quad e(k, z, \overline{z}) = e^{ikz-i\frac{\alpha^2}{k}z}.
\]
A. The Analysis of the Global Relation

Eqs. (2.3) express $\rho_j(k)$ in terms of the unknown functions $\varphi(-ik)$, $\varphi(k)$, and $\psi(+)$. These functions satisfy the global condition: $\sum_{j=1}^{3} \rho_j(k) = 0$. This equation, and its complex conjugate, are

$$\begin{align*}
\alpha(k)\varphi(-ik) + \alpha(-ik)\varphi(k) + E(k)\psi(+) &= F(k) + F(-ik), \quad k \in \mathbb{C}, \\
\alpha(k)\varphi(ik) + \alpha(ik)\varphi(-k) + E(k)\psi(-) &= F(k) + F(ik), \quad k \in \mathbb{C}.
\end{align*}$$

Eqs. (2.7)–(2.10) are invariant under $k \mapsto -k$, the basic equations. Eqs. (2.7) and (2.8) yield

$$\begin{align*}
\alpha(-ik)\varphi(-k) + \alpha(-k)\varphi(-ik) + E(-ik)\psi(-) &= F(-ik) + F(-k), \quad k \in \mathbb{C}, \\
\alpha(ik)\varphi(-k) + \alpha(-k)\varphi(ik) + E(ik)\psi(+) &= F(ik) + F(-k), \quad k \in \mathbb{C}.
\end{align*}$$

Eqs. (2.7)–(2.10) are invariant under $k \mapsto -k$, thus we do not obtain any additional equations using this transformation. Eqs. (2.7)–(2.10) are the basic equations needed for the determination of the unknown functions $\varphi(k)$, $\varphi(-ik)$, $\psi(+)$. The analysis of the basic equations leads to a matrix Riemann-Hilbert problem. However, in what follows we will show that this problem can be bypassed, and that $q(x, y)$ can be obtained using only algebraic manipulations of the basic equations.

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The known functions give rise to the contribution

\[ \sum_{i=1}^{3} \mathcal{G}(k) \mathcal{F}(k) \]

Replacing in this equation $\varphi(ik)$ by Eq. (2.8), and comparing with Eq. (2.7) we find Eq. (2.11). Replacing $\psi(+)$. The analysis of the basic equations leads to a matrix Riemann-Hilbert problem. However, in what follows we will show that this problem can be bypassed, and that $q(x, y)$ can be obtained using only algebraic manipulations of the basic equations.
\[ G(x, y) = \frac{1}{2\pi} \int_{t_1} e(k, z, \zeta) [\alpha(k)G_1(k) - F(-ik)] \frac{dk}{k} + \frac{1}{2\pi} \int_{t_2} e(k, z, \zeta) [\alpha(-ik)G_2(k) - F(k)] \frac{dk}{k} + \frac{1}{2\pi} \int_{t_3} e(k, z, \zeta) E(k)G_3(k) \frac{dk}{k}. \] (2.15)

In what follows we will show that, by using appropriate contour rotations, the integrals involving the functions \( \varphi(ik) \), \( \psi(-) \) can be evaluated in terms of residues. Furthermore, these residues can be computed in terms of the functions \( G_j(k) \). For the justification of these rotations we use the following facts (see Figure 3).

1. \( e(k, z, \zeta), e(k, z, \zeta)E(k), e(k, z, \zeta)E(-ik) \), are bounded for \( 0 < \arg k < \frac{\pi}{2}, \frac{3\pi}{4} < \arg k < \frac{5\pi}{4}, \frac{5\pi}{4} < \arg k < 2\pi \), respectively.
2. If \( E(-k)E(ik) \) and \( \psi(-) \) are bounded for \( -\frac{\pi}{2} < \arg k < \frac{\pi}{2} \), then \( E(ik)E(-ik)\psi(-) \) is bounded for \( \frac{3\pi}{2} < \arg k < \frac{3\pi}{2} \). Hence exp\([\varphi(ik)E(k)E(-ik)\psi(-)] \) can be evaluated in terms of residues. Furthermore, these residues can be computed in terms of the functions \( e(k, z, \zeta)E(k) \). Similar considerations apply to \( e(k, z, \zeta)E(-ik) \).
3. The definition of \( \Delta(k) \) is exponentially small, and \( \varphi(ik)E(k)E(-ik)\psi(-) \) is exponentially large at \( k = 0 \) and \( k = \infty \); using \( z_3 = iL \), this exponential equals \( e(k, z, \zeta)E(k) \). Similar considerations apply to \( e(k, z, \zeta)E(-ik) \).

The contribution of the integral along \( t_3 \), due to the terms involving \( \psi(-) \) (see Eq. (2.11)), gives rise to two integrals: one involving \( e(k, z, \zeta)A(k)E(-ik)E(k)\psi(-)k\Delta(k) \), and one involving \( e(k, z, \zeta)A(-ik)E(k)^2/k\Delta(k) \). The first integral is bounded in \( \frac{3\pi}{2} < \arg k < 2\pi \), while the second integral is bounded in \( \frac{5\pi}{4} < \arg k < \frac{5\pi}{4} \). Indeed, the integrand of the first integral is dominated by\[ [e(k, z, \zeta)E(-ik)]E(k)E(-ik)\psi(-), \quad \frac{3\pi}{2} < \arg k < \frac{3\pi}{2}; \quad [e(k, z, \zeta)E(-ik)]E(k)\psi(-), \quad \frac{5\pi}{4} < \arg k < 2\pi, \] and each of the brackets is bounded. Similarly, the integrand of the second integral is dominated by\[ [e(k, z, \zeta)E(k)]\psi(-), \quad \frac{3\pi}{2} < \arg k < \frac{3\pi}{2}; \quad [e(k, z, \zeta)E(k)]E(k)E(-ik)\psi(-), \quad \frac{5\pi}{4} < \arg k < \frac{5\pi}{4}, \] and each of the brackets is bounded.

Hence, the integral along \( t_3 \), due to the terms involving \( \psi(-) \), equals an integral along \( t_1 \) involving \( e(k, z, \zeta)A(k)E(-ik)E(k)\psi(-)k\Delta(k) \), an integral along \( t_2 \) involving \( e(k, z, \zeta)A(-ik)E(k)^2/k\Delta(k) \), and a contribution due to residues which can be computed below (see Eqs. (2.10a), (2.10b)). Combining these integrals with the integrals due to \( \varphi(-ik) \) and to \( \varphi(k) \) (see Eqs. (2.11a) and (2.11b)), we find
\[ J_1(x, y) = \frac{1}{2\pi} \int_{-\ell_2 \cup \ell_1} e(k, z, \zeta)\left[\frac{1}{2}q(0, 0) + \alpha(k)A(-ik)\varphi(ik)\right] \frac{dk}{k}, \] (2.16)
\[ J_2(x, y) = \frac{1}{2\pi} \int_{-\ell_2 \cup \ell_1} e(k, z, \zeta)A(k)A(-ik)^2E(k)E(ik)\psi(-) \frac{dk}{k}. \] (2.17)

For \( k \) in the first quadrant of the complex \( k \)-plane, \( E(k)/\Delta(k) \) is dominated by 1, and each of the terms \( e(k, z, \zeta), \varphi(ik), E(ik), \psi(-) \) is bounded. Thus, both \( J_1 \) and \( J_2 \) can be computed in terms of residues.

The definition of \( A(k) \) implies\[ A(-ik) = -\frac{(k + \Lambda_1)(k + \Lambda_2)}{(k - \Lambda_1)(k - \Lambda_2)}, \quad A(k) = -\frac{(k + \Lambda_1)(k - \Lambda_2)}{(k - \Lambda_1)(k + \Lambda_2)}, \quad \Lambda_1 = \frac{\gamma}{4}(1 + i), \quad \Lambda_2 = \frac{\gamma}{4}(-1 + i), \] so the poles of \( A(-ik) \) and \( A(k) \) occur at \( \Lambda_1, \Lambda_2 \) and at \( -\Lambda_1, -\Lambda_2 \), respectively. Similarly, the poles of \( A(ik) \) and \( A(-k) \) occur at \( -\Lambda_1, -\Lambda_2, \) and \( -\Lambda_1, \Lambda_2 \), respectively. Using these facts it follows that\[ q(x, y) = G(x, y) + \sum_{j=1}^{3} R_j(x, y) + P(x, y), \] (2.18)
where \(G(x, y)\) is defined by Eq. (2.15), \(P(x, y)\) is the contribution to \(J_1\) and \(J_2\) due to the poles of \(\alpha(k)A(-ik)\) and of \(A(k)\) are defined as follows:

\[
R_1 = i \sum_j \frac{e(\kappa_j, z, \bar{\tau})A(\kappa_j)A(-ik_j)^2E(\kappa_j)E(ik_j)}{\kappa_j \Delta'(\kappa_j)} \psi(\kappa_j) ,
\]

\[
R_2 = -i \sum_j \frac{e(\lambda_j, z, \bar{\tau})A(-\lambda_j)E(\lambda_j)^2}{\lambda_j \Delta'(\lambda_j)} \psi(\lambda_j) + 2 \frac{e(\Lambda_2, z, \bar{\tau})}{\Delta(\Lambda_2)} E(\Lambda_2)^2 \psi(\Lambda_2) ,
\]

\[
R_3 = -i \sum_j \frac{e(\mu_j, z, \bar{\tau})A(\mu_j)E(-i\mu_j)E(\mu_j)}{\mu_j \Delta'(\mu_j)} \psi(\mu_j) - 2 \frac{e(-\Lambda_2, z, \bar{\tau})}{\Delta(-\Lambda_2)} E(-\Lambda_2)E(i\Lambda_2)\psi(-\Lambda_2) ,
\]

\(\psi(k), \Delta'(k)\) denote

\[
\psi(k) = \psi(-ke^{-i\pi/4}) , \quad \Delta'(k) = \frac{d\Delta(k)}{dk} ,
\]

and \(\kappa_j, \lambda_j, \mu_j\) denote the zeros of \(\Delta(k)\) in \(0 < \arg k < \frac{\pi}{4}, \frac{\pi}{4} < \arg k < \frac{5\pi}{4}, \frac{5\pi}{4} < \arg k < 2\pi\), respectively. Multiplying Eq. (2.11b) by \(\Delta(k)\) and evaluating the resulting expression at \(k_j = \{\kappa_j, \lambda_j, \mu_j\}\), we find

\[
\psi(k_j) = -\frac{[1 - A(k_j)][F(-ik_j) - A(-ik_j)F(ik_j)]}{\delta(k_j)} \psi(k_j) + \frac{[1 - A(-ik_j)][F(k_j) - A(k_j)F(-k_j)]}{\delta(k_j)} , \quad \delta(k_j) \neq 0 ,
\]

where

\[
\delta(k) = A(-ik)E(k) + A(k)E(-ik) ,
\]

Noting that \(\alpha(k) = (k + \Lambda_1)(k - \Lambda_2)/2k, \alpha(ik) = -(k - \Lambda_1)(k - \Lambda_2)/2ik\), and evaluating Eq. (2.18) at \(k = \Lambda_2\), we find

\[
\psi(\Lambda_2) = E(-\Lambda_2)[F(\Lambda_2) + F(i\Lambda_2)] , \quad \psi(-\Lambda_2) = E(-i\Lambda_2)[F(\Lambda_2) + F(i\Lambda_2)] .
\]

The term \(P(x, y)\) arises from \(\alpha(k)A(-ik)\) in \(J_1\), and \(A(k)A(-ik)/\Delta(k)\) [\(\Delta(k) \neq 0\)] in \(J_2\), each of which has a simple pole at \(k = \Lambda_1\). Evaluation of the pertaining residues yields

\[
P(x, y) = 2e(\Lambda_1, z, \bar{\tau})[\alpha(\Lambda_1)\varphi(\Lambda_1) + E(\Lambda_1)\psi(\Lambda_1)] .
\]

Evaluating Eq. (2.8) at \(k = \Lambda_1\), we find

\[
\alpha(\Lambda_1)\varphi(\Lambda_1) + E(\Lambda_1)\psi(\Lambda_1) = F(\Lambda_1) + F(i\Lambda_1) .
\]

Thus,

\[
P(x, y) = 2e(\Lambda_1, z, \bar{\tau})[F(\Lambda_1) + F(i\Lambda_1)] .
\]

**In summary:** Assume that \(\delta(k_j) \neq 0\), where \(k_j\) is a zero of \(\Delta(k)\), and \(\delta(k), \Delta(k)\) are defined by Eqs. (2.12b), (2.22), respectively. Then \(q(x, y)\) is given by Eq. (2.18), where \(G(x, y)\) is defined by Eq. (2.13), \(P(x, y)\) is defined by Eq. (2.22), and \(R_j(x, y), j = 1, 2, 3\), are defined by Eqs. (2.16), with \(\psi(k_j), \psi(\Lambda_2), \psi(-\Lambda_2)\) defined by Eqs. (2.21), (2.23).

**III. THE PHYSICAL PROBLEM**

The physical problem corresponds to the homogeneous BCs, i.e., \(f = 0\). In this case Eq. (2.18) yields \(q(x, y) = 0\). Thus, we only need to consider the assumption that \(\delta(k_j) \neq 0\). If this assumption is violated then the equations \(\Delta(k) = 0\) and \(\delta(k) = 0\) can be rewritten in the form

\[
A(ik_n)^2E(-ik_n)^2 = 1 ,
\]

\[
A(-k_n)^2E(k_n)^2 = 1 .
\]

Eqs. (3.1) do not have a solution for generic values of \(\gamma\). Indeed, consider first the limit of infinite back reaction rate, \(\gamma L \to \infty\). Inspection of Eqs. (3.1) in this limit yields the asymptotic solution \(k_\infty = \pm \Lambda_1, \pm \Lambda_2\). If there exists
a steady state other than $q(x,y) = 0$, then it would also exist for $\gamma L$ large but finite. We therefore seek solutions of (3.3) of the form $k = k_\infty + \epsilon$. Such solutions do not exist: Using $k_\infty = \Lambda_1$, Eq. (3.1b) yields $\epsilon = \frac{L}{4\beta}(-1 + i)$ — to first order in $\epsilon$ — while Eq. (3.1b) yields the contradictory result $\epsilon = \frac{1}{4\beta}(1 + 1 - i)$. The other values of $k_\infty$ lead to similar contradictory results. Thus, the only solution to the physical problem is $q(x,y) = 0$, which corresponds to the trivial case of the vacuum; when no particles are left in the system.

Finally, consider the relaxation of the system into the absorbing empty state. Instead of Eq. (1.2), we need to study

$$E_{xx} + E_{yy} + \gamma(-E_x + E_y) = E_\tau,$$

where $\tau = D\tau$ is a rescaled time parameter. We turn this into an eigenvalue problem, by writing $E(x,y,t) = 1 - e^{-\sigma \tau} e^{-\gamma(y-x)}q_\sigma(x,y)$. This results in an equation for $q_\sigma$ identical to Eq. (1.2), valid over the same domain, but with $4\beta^2 = \frac{1}{2}\gamma^2 - \sigma$. The BCs for this equation are identical to (1.3). We have already seen that the problem admits no zero eigenvalue: $q_0(x,y) = 0$. The analysis for $\sigma > 0$ proceeds along the same lines. Once again, the critical issue is whether there exist solutions of Eqs. (1.3). This time the asymptotic solution for $\gamma L \to \infty$ is $k_\infty = \frac{2}{\gamma}\sqrt{\pm[1 \pm \sqrt{1 - \frac{4\beta}{\gamma^2}}]}$, $\gamma L < 1$, provided that $\sigma \sim 2\gamma^2 e^{-\gamma L/2}$. The relaxation time to the empty state is therefore $(D\sigma)^{-1} = (D/2\nu^2)e^{\nu L/2D}$.

It is instructive to compare our analysis of $A + A \rightleftharpoons A$ to the mean-field result. The reaction-diffusion equation for the steady state of the process, in a segment demarcated by traps, is

$$D\rho_{xx} + k_1\rho - k_2\rho^2 = 0, \quad -L/2 \leq x \leq L/2,$$

where $\rho(x)$ is the local particle density, $k_1$ is the rate of the back reaction $A \to A + A$, $k_2$ is the rate of $A + A \to A$, and the traps impose the BCs $\rho(\pm L/2) = 0$. This equation predicts a transition from an empty state ($\rho = 0$) to an active state ($\rho > 0$), when $k_1$ exceeds a certain critical value [8]. Our exact analysis shows that in the actual system of one-dimensional coalescence the noise destroys the transition and the only existing steady state is the empty state. The nontrivial steady state of the mean-field case is echoed in the exponentially large relaxation time found for large back reaction rates. Although the lack of a transition cannot be established from numerical simulations, especially in view of the long relaxation times for $\gamma L$ large, previous work had suggested that a transition does not take place [9].

ACKNOWLEDGMENTS

We thank Prof. L. Glasser and Prof. D. Kessler for useful discussions, and Prof. A. C. Newell for important suggestions. We gratefully acknowledge the NSF (D.b.-A.) and the EPRSC (A.S.F.) for support of this work.
FIG. 1. Domain of the modified Helmholtz equation, Eq. (1.2).

FIG. 2. The rays $\ell_j$, in the complex plane, along which $q(x,y)$ is computed (Eq. (2.1)).

FIG. 3. Regions where $e(k,z,\bar{z})$, $e(k,z,\bar{z})E(k)$, $e(k,z,\bar{z})E(-ik)$, $\psi(-)$, $E(k)E(-ik)\psi(-)$ are bounded, and dominant behavior of $\Delta(k)$. 