

THE STRUCTURE OF THE PERTURBATION FRONT IN TRANSPORT PROCESSES WITH RELAXATION†

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In a study of transport processes with a relaxation kernel of general form, the distribution of the transported quantity is determined near a front created by perturbations emerging from a point source. This is the region in which the specific form of the kernel function becomes significant, since at a distance from the front the process is adequately described by the heat-conduction equation. General physical and thermodynamic conditions that must be imposed on the relaxation kernel are formulated. The distribution near the front is computed separately in one, two and three dimensions.

IT IS WELL known that transport processes of very diverse kinds (heat conduction, diffusion, propagation of transverse modes in a viscous fluid, filtering, etc.) are governed by parabolic equations similar to the heat-conduction equation. These equations allow the velocity at which the signal propagates to become infinite, contrary to the principles of modern physics, since the velocity of propagation of a signal can never exceed the speed of light in a vacuum. Therefore, for a physically consistent theory of transport processes, one must modify the basic dynamical equation. One proposal [1] is to replace the parabolic equation by a hyperbolic one. It was later realized that the results in [1] are a special case of a more general approach, which takes into account the relaxation relationship between the flow of the transported quantity and its gradient [2]. This relationship arises quite naturally in kinetic theory and non-equilibrium statistical mechanics [3]. The question of the limiting velocity of a signal has been investigated [4] for a relaxation kernel of general form.

1. Consider a homogeneous, isotropic medium at rest, with an attached reference frame t, x^1, x^2, x^3 , where x^1, x^2, x^3 are Cartesian coordinates. Suppose that some physical quantity $u = u(t, x^i)$ (e.g. the temperature, the concentration of an impurity, etc.) can be transported in the medium. Let us assume that at equilibrium u takes a constant value, defined by the boundary conditions. We may assume without loss of generality that this value is zero. The dynamics of $u(t, x^i)$ are described by the equation

$$u_t + \nabla \mathbf{J} = q \quad (1.1)$$

Here \mathbf{J} is the flow vector of u and $q = q(t, x^i)$ is the field of the sources. For a homogeneous isotropic medium \mathbf{J} is usually taken as

$$\mathbf{J} = -\kappa \nabla u \quad (1.2)$$

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where $\kappa = \text{const} > 0$ is the transport coefficient. If (1.2) is substituted into Eq. (1.1), the latter reduces to the heat-conduction equation

$$u_t - \kappa \Delta u = q \tag{1.3}$$

where Δ is the Laplacian. According to (1.3), perturbations of the field $u = u(t, x^i)$ will propagate at infinite velocity. As shown in [4], the paradox of an infinite signal propagation velocity may be eliminated by replacing (1.2) with the more-general relaxation relation

$$\mathbf{J}(t, x^i) = -\kappa \int_{-\infty}^{+\infty} K(t-t') \nabla u(t', x^i) dt' \tag{1.4}$$

The kernel $K = K(t)$ is independent of the space coordinates; it describes intrinsic relaxation processes in the medium. The function $K = K(t)$ must satisfy various conditions, of a physical and thermodynamic nature.

Following [4, 5], we will list these conditions.

If ∇u varies with time, maintaining a constant direction at a given point in space, it is natural to assume that the corresponding flow \mathbf{J} has the opposite direction at that point at all times. This is equivalent to the following conditions.

Condition 1. $K = K(t)$ is a non-negative function with the dimensions of $(\text{time})^{-1}$.

The ∇u is constant in time, Eq. (1.4) must reduce to (1.2), so that

Condition 2. $\int_{-\infty}^{+\infty} K(t) dt = 1$

The kernel $K = K(t)$ describes the effect of the field ∇u on \mathbf{J} . By the causality principle, $\nabla u(t', x^i)$ cannot affect $\mathbf{J}(t, x^i)$ if $t' > t$. Therefore $K(t) = 0$ if $t < 0$. If $t > t'$ then, $t - t'$ increases, the effect of $\nabla u(t', x^i)$ on $\mathbf{J}(t, x^i)$ should diminish, that is, $K(t)$ must be a decreasing function. Furthermore, by [4] the maximum signal velocity of propagation in models (1.1) and (1.4) is $v = (\kappa K(0))^{1/2}$. We shall assume that it is finite.

Let $S[a, b]$ denote the space of rapidly decreasing functions in the interval $[a, b]$, where possibly $a = -\infty$ or $b = +\infty$, i.e. the space of real infinitely differentiable functions $f = f(t)$ in $[a, b]$ with the topology defined by the denumerable set of seminorms

$$\|f\|_{m, n} = \sup_{t \in [a, b]} \left| t^m \frac{d^n f}{dt^n}(t) \right|; \quad n, m = 0, 1, 2, \dots$$

Let $S'[a, b]$ denote the space of functions dual to $S[a, b]$, i.e. the space of continuous linear functionals in $S[a, b]$.

In view of the above remarks, we will adopt the following assumption.

Condition 3. The support of $K = K(t)$ is a subset of the half-line $[0, +\infty)$, $K|_{[0, +\infty)} \in S[0, +\infty)$ and $K|_{[0, +\infty)}$ is a monotone decreasing function.

We will now consider the quantity

$$W(x^i) = - \int_{-\infty}^{+\infty} \nabla u(t, x^i) \mathbf{J}(t, x^i) dt$$

for any sequence $\partial u / \partial x^j(\cdot, x^i) \in S[-\infty, +\infty]$. In any transport process, $W(x^i)$ is proportional to the

total entropy produced in a particle x^i of the medium in a closed thermodynamic cycle. By the Second Law of Thermodynamics, $W(x^i)$ is always non-negative.

Using formula (1.4), we get the following.

Condition 4. For any function $f \in S[-\infty, +\infty]$,

$$\int_{-\infty}^{+\infty} dt_1 \int_{-\infty}^{+\infty} dt_2 K(t_1 - t_2) f(t_1) f(t_2) \geq 0$$

Henceforth, the Fourier transform of any function $f \in S'[-\infty, +\infty]$ will be denoted by $f_F = f_F(\omega)$:

$$f_F(\omega) = \int_{-\infty}^{+\infty} e^{-i\omega t} f(t) dt$$

Conditions 1–4 have various implications about the Fourier transform of the kernel, $K_F(\omega)$.

Following [5], we will list three results here.

$K_F = K_F(\omega)$ is holomorphic in the lower complex half-plane ω and continuous up to the real axis.

Moreover, $K_F(0) = 1$, $\overline{K_F(\omega)} = K_F(-\bar{\omega})$, where $\text{Im } \omega \leq 0$ and

$$|K_F(\omega)| \leq 1, \text{Im } \omega = 0 \quad (1.5)$$

In terms of Fourier transforms, condition 4 is equivalent to

$$\int_0^{+\infty} |f_F(\omega)|^2 \text{Re } K_F(\omega) d\omega \geq 0$$

Hence, since $f_F(\omega)$ is arbitrary for $\omega \geq 0$, it follows that $\text{Re } K_F(\omega)$ is non-negative. The fact is that if $\text{Re } K_F(\omega_0)$ were to vanish, this would imply the possibility of a non-dissipative oscillatory process at a frequency ω_0 . This is indeed what happens in superfluids and superconductors. We shall exclude this case, imposing the more stringent condition

$$\text{Re } K_F(\omega) > 0, \omega \in R \quad (1.6)$$

As $|\omega| \rightarrow +\infty$ one has the asymptotic expansion

$$K_F(\omega) = \sum_{n=1}^{+\infty} k_{-n} (i\omega)^{-n}, \quad k_{-n} = \left. \frac{d^{n-1} K}{dt^{n-1}} \right|_{t=+\infty} \quad (1.7)$$

In view of (1.6), we will require here that $k_{-2} < 0$. Since $K_F(\omega) \rightarrow 0$ as $|\omega| \rightarrow +\infty$, it follows from (1.5), (1.6) and the general theory [6, 7] that the complex function $K_F = K_F(\omega)$ maps the half-plane $\text{Im } \omega < 0$ onto some domain in the disk $|z| < 1$, $\text{Re } z > 0$, $z \in C$.

2. Equations (1.1) and (1.4) yield an integrodifferential equation

$$u_t(t, x^i) - \kappa \int_{-\infty}^{+\infty} K(t - t') \Delta u(t', x^i) dt' = q(t, x^i)$$

which, in terms of Fourier transforms, may be written as

$$(\Delta - \alpha^2) u_F = -q_F / (\kappa K_F) \quad (2.1)$$

Here $u_F = u_F(\omega, x^i)$, $q_F = q_F(\omega, x^i)$ and α is a complex quantity, defined by

$$\alpha^2 = i\omega / (\kappa K_F), \text{Re } \alpha \geq 0 \quad (2.2)$$

We will show that these relations in fact define a function $\alpha = \alpha(\omega)$ which is holomorphic in the lower complex half-plane and satisfies the strict inequality

$$\operatorname{Re} \alpha(\omega) > 0, \operatorname{Im} \omega \leq 0, \omega \neq 0 \tag{2.3}$$

Indeed,

$$\operatorname{Im} K_F = - \int_0^{+\infty} e^{t \operatorname{Im} \omega} \sin(t \operatorname{Re} \omega) K(t) dt \tag{2.4}$$

It follows from (2.4) and Condition 3 that

$$-\operatorname{Re} \omega \operatorname{Im} K_F \geq 0 \tag{2.5}$$

Next,

$$\operatorname{Im} (i\omega/K_F) = (\operatorname{Re} \omega \operatorname{Re} K_F + \operatorname{Im} \omega \operatorname{Im} K_F) / |K_F|^2 \tag{2.6}$$

The results of Sec. 1, (2.6), (2.5) and (2.2) imply (2.3). Using (2.2) and (1.7) we obtain an asymptotic expansion as $|\omega| \rightarrow +\infty$:

$$\begin{aligned} \alpha(\omega) &= \sum_{n=-1}^{+\infty} a_{-n} (i\omega)^{-n}, \quad a_1 = (\kappa k_{-1})^{-1/2} = \nu^{-1}, \\ a_0 &= -2^{-1} \kappa^{-1/2} k_{-1}^{-3/2} k_{-2}, \\ a_{-1} &= -2^{-1} \kappa^{-1/2} k_{-1}^{-3/2} k_{-3} + 3 \cdot 2^{-3} \kappa^{-1/2} k_{-1}^{-3/2} k_{-2}^2, \dots \end{aligned} \tag{2.7}$$

We shall consider the problem of the propagation of perturbations from a point source separately in one, two or three dimensions. The number of dimensions will be characterized by a parameter ν ($\nu = 1, 2, 3$). We write

$$q = Q(t) \prod_{i=1}^{\nu} \delta(x^i)$$

and the dependence of u_F on the coordinates reduces to a dependence on

$$r = \left(\sum_{i=1}^{\nu} (x^i)^2 \right)^{1/2}.$$

Substituting the expressions for the Laplacian $\Delta = \partial^2/\partial r^2 + (\nu-1)r^{-1} \partial/\partial r$ into (2.1), we obtain

$$u_F = Q_F J_0, \quad J_0 = J_0(\omega, r) = (\kappa K_F)^{-1} (2\pi)^{-\nu/2} (r/\alpha)^\lambda K_\lambda(\alpha r)$$

where $\lambda = (2-\nu)/2$, $K_\lambda = K_\lambda(z)$ is the Macdonald function [8, 9]. We know that

$$K_{\pm 1/2}(z) = \sqrt{\frac{\pi}{2z}} e^{-z} \tag{2.8}$$

and we have the following asymptotic expansions for $\omega \rightarrow 0$ (C is Euler's constant):

$$K_0(z) = \ln(z\gamma/2) + O(z^2 \ln z), \quad \gamma = e^C \tag{2.9}$$

and as $|\omega| \rightarrow +\infty$:

$$K_0(z) = \sqrt{\frac{\pi}{2z}} e^{-z} \sum_{m=0}^{+\infty} \frac{\Gamma(1/2 + m)}{m! \Gamma(1/2 - m)} (2z)^{-m} \tag{2.10}$$

Macdonald's functions are analytic throughout the complex plane cut along the negative real axis.

Let $N \geq 2$ be a natural number, y_j ($j = 1, \dots, N + 1$) an arbitrary sequence of pairwise distinct positive numbers and $X_j = X_j(r)$ ($j = 1, \dots, N + 1$) a sequence of functions of r , which will be defined later on for each specific value of ν . Define functions

$$F_1 = F_1(\omega) = \sum_{j=1}^{N+1} \frac{x_{j1}}{i\omega + y_j}, \quad F_2 = F_2(\omega) = \sum_{j=1}^{N+1} \frac{x_{j2}}{i\omega + y_j} + x_{02}$$

such that the coefficients x_{j1}, x_{j2} satisfy the systems of equations

$$\sum_{j=1}^{N+1} x_{j1} y_j^{-1} = 1, \quad \sum_{j=1}^{N+1} x_{j1} y_j^k = 0, \quad k = 0, \dots, N - 1 \tag{2.11}$$

$$x_{02} + \sum_{j=1}^{N+1} x_{j2} y_j^{-1} = 0, \quad x_{02} = X_0 \tag{2.12}$$

$$\sum_{j=1}^{N+1} x_{j2} y_j^k = (-1)^k X_{k+1}, \quad k = 0, \dots, N - 1$$

Systems (2.11) and (2.12) always have unique solutions.

To simplify matters, we will set $Q(t) = A\theta(t)$, where $\theta(t)$ is the Heaviside function. Then $Q_F(\omega) = A(i\omega + \varepsilon)^{-1}$, where ε is a small positive number, to be set equal to zero in the final result.

Let $\nu = 1$.

Letting $\omega \rightarrow 0$ in (2.8), we obtain the asymptotic formula

$$J_0 = \lambda_1 (i\omega)^{-1/2} + \lambda_2 + O(|\omega|^{1/2}), \quad \lambda_1 = -2^{-1} \kappa^{-1/2},$$

$$\lambda_2 = -2^{-1} \kappa^{-1/2} r \tag{2.13}$$

We shall regard $z^{1/2}$ as an analytic function in the complex plane cut along the negative real axis. Using (2.7) and (2.8) we obtain the following asymptotic expansion for $|\omega| \rightarrow +\infty$:

$$J_0 = e^{-i\omega r/\nu} \sum_{n=0}^{+\infty} X_n(r) (i\omega)^{-n} \tag{2.14}$$

$$X_0 = (2\kappa k_{-1} a_1)^{-1} e^{-ra_1}, \quad X_1 = -X_0 \left(ra_{-1} + \frac{k_{-2}}{2k_{-1}} \right), \dots$$

Define a new function $J_1 = J_1(\omega, r)$ by

$$J_0 = e^{-i\omega r/\nu} (J_1 + (\lambda_1 (i\omega)^{-1/2} + \lambda_2) F_1 + F_2) \tag{2.15}$$

Formulas (2.11) and (2.14) imply the asymptotic relation $J_1 = O(|\omega|^{1/2})$ as $\omega \rightarrow 0$, $J_1 = O(|\omega|^{-(N+1)})$ as $|\omega| \rightarrow +\infty$. From (2.15) we obtain the representation

$$u(t, r) = u_1(t, r) + u_2(t, r) \tag{2.16}$$

$$u_1(t, r) = \frac{A}{2\pi} \int_{-\infty}^{+\infty} e^{i\omega\tau} ((\lambda_1 (i\omega)^{-1/2} + \lambda_2) F_1 + F_2) \frac{d\omega}{i\omega + \varepsilon}$$

$$u_2(t, r) = \frac{A}{2\pi} \int_{-\infty}^{+\infty} e^{i\omega\tau} (i\omega)^{-1} J_1 d\omega$$

where $\tau = t - r/v$. Using Lebesgue's convergence theorem, one can show that $u_2(r, t)$ is N times continuously differentiable. Since $u_2(t, r) = 0$ if $\tau < 0$ (the Paley-Wiener Theorem [7]), it follows that $u_2 = o(\tau^N)$ if $\tau \geq 0$. Evaluation of $u_1(t, r)$ by using the identity

$$(i\omega + y)^{-1} (i\omega + \varepsilon)^{-1} = (y - \varepsilon)^{-1} [(i\omega + \varepsilon)^{-1} - (i\omega + y)^{-1}] \tag{2.17}$$

reduces to evaluating integrals of the type

$$I_1 = \int_{-\infty}^{+\infty} \frac{e^{i\omega\tau} d\omega}{(i\omega)^{1/2} (i\omega + y)}, \quad I_2 = \int_{-\infty}^{+\infty} e^{i\omega\tau} (i\omega + y)^{-1} d\omega \quad (y > 0)$$

The integral I_1 is evaluated by deforming the contour of integration to the two sides of a cut by using formula 3.466.1 in [9], while I_2 can be evaluated by using the Residue Theorem. We obtain

$$I_1 = -2\pi i y^{1/2} \Phi(i(y\tau)^{1/2}) e^{-y\tau} \theta(\tau), \quad I_2 = 2\pi e^{-y\tau} \theta(\tau)$$

where $\Phi(z)$ is the probability integral. Expanding Φ in series in terms of τ , as in formula 8.253.1 of [9], we obtain

$$u = \left(A \sum_{n=0}^N X_n \frac{\tau^n}{n!} + o(\tau^N) \right) \theta(\tau) \tag{2.18}$$

Now let $\nu = 2$.

Formulas (2.9), (2.7) and (2.10) yield

$$\begin{aligned} \omega \rightarrow 0, \quad J_0 &= \lambda_3 \ln((i\omega)^{1/2} \gamma/2) + O(|\omega| \ln|\omega|), \\ \lambda_3 &= (2\pi\kappa)^{-1} \end{aligned} \tag{2.19}$$

$$|\omega| \rightarrow +\infty, \quad J_0 = e^{-i\omega r/v} (i\omega)^{1/2} \sum_{n=0}^{+\infty} X_n(r) (i\omega)^{-n} \tag{2.20}$$

$$X_0 = (2\pi\kappa a_1 k_{-1})^{-1} (\pi/2r)^{1/2} e^{-ra_1}$$

$$X_1 = -X_0 \left(\frac{3k_{-2}}{4k_{-1}} + ra_{-1} + \frac{1}{8ra_1} \right), \dots$$

We will define a function $J_2 = J_2(\omega, r)$ by the formula

$$J_0 = e^{-i\omega r/v} (J_2 + \lambda_3 \ln((i\omega)^{1/2} \gamma/2) F_1 + (i\omega)^{1/2} F_2) \tag{2.21}$$

Formulas (2.19) and (2.20) imply the asymptotic relations $J_2 = O(|\omega| \ln|\omega|)$ as $\omega \rightarrow 0$ and $J_2 = O(|\omega|^{-[N+(1/2)]})$ as $|\omega| \rightarrow +\infty$.

Formula (2.21) implies the representation (2.16) with

$$u_1(t, r) = \frac{A}{2\pi} \int_{-\infty}^{+\infty} e^{i\omega\tau} (\lambda_3 \ln((i\omega)^{1/2} \gamma/2) F_1 + (i\omega)^{1/2} F_2) \frac{d\omega}{i\omega + \varepsilon}$$

$$u_2(t, r) = \frac{A}{2\pi} \int_{-\infty}^{+\infty} e^{i\omega\tau} (i\omega)^{-1} J_2 d\omega$$

As before, it can be proved that $u_2(t, r) = 0$ if $\tau < 0$ and $u_2(t, r) = o(\tau^N)$ if $\tau \geq 0$. Evaluation of u_1 using the identity (2.17) reduces to evaluating integrals of the type I_2 , and also

$$I_3 = \int_{-\infty}^{+\infty} \frac{\ln(i\omega)^{1/2} e^{i\omega\tau}}{i\omega + y} d\omega, \quad I_4 = \int_{-\infty}^{+\infty} \frac{(i\omega)^{1/2} e^{i\omega\tau}}{i\omega + y} d\omega \quad (y > 0)$$

These integrals are evaluated by deforming the contour of integration to the two sides of a cut, using formulas 3.352.6 and 3.466.2 of [9]. The results are

$$I_3 = \pi e^{-y\tau} (\ln y - \text{Ei}(y\tau)) \theta(\tau) \\ I_4 = [2\pi^{1/2}\tau^{-1/2} + 2\pi i y^{1/2} e^{-\tau y} \Phi(i(y\tau)^{1/2})] \theta(\tau)$$

Here $\text{Ei}(z)$ is the integral exponential function.

Using formulas for the series expansions of $\text{Ei}(z)$ and $\Phi(z)$ (formulas 8.214.2 and 8.253.1 in [9]), we finally obtain

$$u = \left(A\pi^{-1/2}\tau^{-1/2} \sum_{n=0}^{\infty} \frac{2^n X_n}{(2n-1)!!} \tau^n + o(\tau^N) \right) \theta(\tau) \quad (2.22)$$

Let $\nu = 3$.

Formulas (2.7) and (2.8) yield

$$\omega \rightarrow 0, \quad J_0 = \lambda_4 + O(|\omega|^{1/2}), \quad \lambda_4 = (4\pi\kappa r)^{-1} \quad (2.23)$$

$$|\omega| \rightarrow +\infty, \quad J_0 = i\omega \sum_{n=0}^{+\infty} X_n(r) (i\omega)^{-n} \quad (2.24)$$

$$X_0 = (4\pi\kappa k_{-1} r)^{-1} e^{-ra_0}, \quad X_1 = -X_0 \left(\frac{k_{-2}}{k_{-1}} + ra_{-1} \right), \dots$$

We define a function J_3 by means of the equation

$$J_0 = e^{-i\omega\tau/\nu} (J_3 + \lambda_4 F_1 + i\omega F_2)$$

Formulas (2.23) and (2.24) imply the asymptotic relations $J_3 = O(|\omega|^{1/2})$ as $\omega \rightarrow 0$ and $J_3 = O(|\omega|^{-N})$ as $|\omega| \rightarrow +\infty$.

Consider the expansion (2.16), where

$$u_1(t, r) = \frac{A}{2\pi} \int_{-\infty}^{+\infty} e^{i\omega\tau} (\lambda_3 F_1 + i\omega F_2) \frac{d\omega}{i\omega + \varepsilon} \\ u_2(t, r) = \frac{A}{2\pi} \int_{-\infty}^{+\infty} e^{i\omega\tau} (i\omega)^{-1} J_3 d\omega$$

Using Lebesgue's convergence theorem, one can prove that $u_2(t, r)$ is $N-1$ times continuously differentiable with respect to t . Since it vanishes when $\tau < 0$ (the Paley-Wiener Theorem [7]), it follows that when $\tau \geq 0$ we have $u_2 = o(\tau^{N-1})$. Evaluation of $u_1(t, r)$ using formula (2.17) reduces to evaluating integrals of type I_2 . Expanding the final result in series we obtain

$$u(t, r) = A \left[X_0 \delta(\tau) + \theta(\tau) \left(\sum_{k=0}^{N-1} X_{k+1} \frac{\tau^k}{k!} + o(\tau^{N-1}) \right) \right] \quad (2.25)$$

3. Formulas (2.18), (2.22) and (2.25) constitute the main result of this paper. They enable one to relate the structure of the perturbation front in a transport process with relaxation to the behaviour

of a relaxation series for small values of the time. In principle, therefore, experimental investigation of the front may yield information about the kernel.

Our main result was derived for a source represented by the Heaviside function $\theta(t)$. Differentiation of formulas (2.18), (2.22) and (2.25) with respect to τ yields formulas for a source represented by the Dirac function $\delta(t)$.

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