

Numerical Treatment of a Boundary-Value Problem for a Certain Singular Parabolic Partial Differential Equation*

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Received July 17, 1985; revised February 26, 1987

We solve a boundary-value problem for a certain linear *singular* partial differential equation of *parabolic* type by a suitable implicit finite-difference scheme. This allows us to obtain precise tabulated values for the mean powers reflected and transmitted by a slab of random medium. This is relevant, e.g., to Plasma Physics. © 1988 Academic Press, Inc.

1. INTRODUCTION

The purpose of this paper is twofold. On the one hand, we want to show how to numerically treat some boundary-value (BV) problems for certain types of *linear singular parabolic* differential equations arising within the context of Probability Theory. To be more precise, these equations represent the Kolmogorov backward equations which describe the evolution of the moments of the complex-valued reflection coefficient, in the linear theory of wave propagation in one-dimensional random media. However, this represents more than a mere example, as several other problems, for instance, problems dealing with linear and nonlinear random oscillators, call for a numerical treatment of "singular" parabolic equations. Furthermore, general theories for BV-problems for parabolic partial differential equations (PDEs), even nonsingular ones, do *not* exist as yet. By a "singular" equation we mean that at least one of the cases of degeneracy, unbounded coefficients or unbounded domain occurs. On the other hand, we want to obtain precise numerical values, to be used in some problems which recently have been proven important within the framework of Plasma Physics; cf. [2].

In Section 2 we briefly outline the underlying physical problem and display the

* This work was supported, in part, by the Air Force Office of Scientific Research, under Grant AFOSR-80-0228, a NATO fellowship, and the U. S. Department of Energy, under Grant DE-FG02-86-ER53223.

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PDE to be solved. In Section 3 we describe the method adopted to carry out such a program and in Section 4 we give an extensive tabulation of the quantity which, in the physical problem, represents the expected value $\langle |R|^2 \rangle$, R being the complex-valued reflection coefficient referred to above. These numerical results will also be discussed regarding convergence, accuracy and stability. The approach of the solution from the initial value to steady state is also discussed. In Section 5, we summarize the important points of the paper.

2. THE ORIGINAL PROBLEM: DERIVATION OF THE PDE

When a plane wave, incoming from a half-space $x > L$, impinges upon a slab of (deterministic or random) medium located in $0 < x < L$ and characterized by the refractive index $n(x) \equiv n_0[1 + \varepsilon g(x)]^{1/2}$, it is, in general, partially transmitted through the slab and partially reflected back.

The scalar wave field, $y^\varepsilon(x)$, satisfies an equation like

$$\frac{d^2 y^\varepsilon}{dx^2} + k_0^2 \left[\frac{n(x)}{n_0} \right]^2 y^\varepsilon = 0, \quad 0 < x < L \quad (2.1)$$

(cf. [5]), plus boundary conditions at $x = 0$ and $x = L$ which state the continuity of y^ε , $y^{\varepsilon'}$ across the slab $[0, L]$. Assuming that the field is

$$y = e^{-ik_0(x-L)} + R^\varepsilon(L) e^{ik_0(x-L)} \quad \text{for } x > L,$$

and

$$y = T^\varepsilon(L) e^{-ik_0 x} \quad \text{for } x < 0, \quad (2.2)$$

the boundary conditions are

$$\begin{aligned} y^\varepsilon(0) &= T^\varepsilon, & y^{\varepsilon'}(0) &= -ik_0 T^\varepsilon \\ & & &= -ik_0 y^\varepsilon(0), \\ y^\varepsilon(L) &= 1 + R^\varepsilon, & y^{\varepsilon'}(L) &= -ik_0(1 - R^\varepsilon) \\ & & &= -ik_0[2 - y^\varepsilon(L)]. \end{aligned} \quad (2.3)$$

Here k_0 represents the vacuum space wave number. As ε is a small real parameter, the refractive index is conceived as a small perturbation around the vacuum value.

The transmission and reflection coefficients, $T^\varepsilon(L)$ and $R^\varepsilon(L)$, are complex-valued quantities which depend on ε and L , the slab-thickness, as well as k_0 and the physical properties of the medium. If the medium neither dissipates nor generates energy, then $|T^\varepsilon|^2 = 1 - |R^\varepsilon|^2$, $|R^\varepsilon|^2$ and $|T^\varepsilon|^2$ being the powers reflected and transmitted by the slab, respectively.

It is well known that $R^\varepsilon(L)$ satisfies the Riccati equation

$$\frac{dR^\varepsilon(L)}{dL} = \varepsilon \frac{ik_0}{2} g(L)(e^{ik_0L}R^\varepsilon(L) + e^{-ik_0L})^2, \quad L > 0, \quad R^\varepsilon(0) = 0, \quad (2.4)$$

when the slab is imbedded in a vacuum space, so that the index of refraction in the half-spaces $x < 0$ and $x > L$ is n_0 (cf., e.g., [7]).

Determining R^ε , $|R^\varepsilon|^2$ (or the corresponding average quantities, when the medium in $0 < x < L$ is random) is perhaps the first important goal in studying the scattering properties of the slab $(0, L)$. On the other hand, handling a Riccati equation such as (2.4) is advantageous from the numerical viewpoint, as in this case we face initial-value (IV) problems (suitable for implementation of iterative computational schemes), while the underlying wave equation is associated with a two-point BV-problem (cf. [7]).

In the *deterministic* case we are done. When the slab is made up of a *random* medium, and therefore $g(x)$ represents a certain stochastic process, we are interested in the *average* value of $|R^\varepsilon|^2$, say $\langle |R^\varepsilon|^2 \rangle$, i.e., the *mean reflected power*. Now, a limit-theorem from the Theory of Stochastic Differential Equations, due to Kahsminskii [4], implies that, under suitable but somewhat general conditions, when $\varepsilon \rightarrow 0$ and $L \rightarrow \infty$, with $\varepsilon^2L \equiv t$ fixed, the random function $R^\varepsilon(\varepsilon^2L)$ will converge (in some weak sense) to some limiting random function, say $R(\varepsilon^2L) \equiv R^0(\varepsilon^2L)$ (diffusion limit). This function represents a *diffusion process* and can be described statistically by the relevant *Fokker-Planck equation* or by its adjoint, the *Kolmogorov backward equation*, which can be explicitly constructed (see the Appendix).

In the case corresponding to (2.4), this last equation has the form

$$\frac{\partial u}{\partial \tau} = (1 - \rho^2)^2 \frac{\partial^2 u}{\partial \rho^2} + \frac{(1 - \rho^2)^2}{\rho} \frac{\partial u}{\partial \rho}, \quad 0 < \rho < 1, \tau > 0. \quad (2.5)$$

Here $\rho \equiv |R|$, $\tau \equiv (k_0^2/8) I_1 t$, $t \equiv \varepsilon^2L$, and

$$I_1 \equiv \int_0^\infty \mathcal{B}(x) \cos(2k_0x) dx \quad (2.5')$$

is essentially the *power spectral density* of the process $g(\cdot)$, $\mathcal{B}(\cdot)$ being its *correlation function*.

Remark. It is worthwhile to observe that the statistical description of our physical phenomenon, resting on (2.5), applies, under very general (statistical) assumptions, on the random function $g(x)$ entering (2.1). The effect of such a “noise” appears in (2.5) via its power spectral density only, which appears as a scaling factor in the variable τ .

Together with the IV $u(\rho, 0) = \rho^2$, Eq.(2.2) allows us to determine $\langle |R(t)|^2 \rangle = u(0, t)$ (cf. (A5), in the Appendix), which we shall take as an approximation to $\langle |R^\varepsilon(\varepsilon^2L)|^2 \rangle$, when ε is small and L is large.

Note that when we construct the infinitesimal generator and then the Kolmogorov backward equation, we get a parabolic operator in *two* space variables, x and y or, in polar coordinates, ρ and ϕ . Independence of ϕ leads to Eq. (2.5).

Note that Eq. (2.5) has one coefficient *singular* as $\sim 1/\rho$ as $\rho \rightarrow 0$, and is *degenerate* at $\rho = 1$, as at that point it is no longer parabolic.

Our purpose is to describe the numerical treatment of the BV-problem associated with Eq. (2.5) and to give precise numerical values of the quantities $\langle |R(t)|^2 \rangle$, $\langle |T(t)|^2 \rangle = 1 - \langle |R(t)|^2 \rangle$, $t \equiv \varepsilon^2 L$, correspondingly to Eq. (2.4), in the diffusion limit referred to above, $\varepsilon \rightarrow 0$, $L \rightarrow \infty$, $\varepsilon^2 L \equiv t$ fixed. The quantity $\langle |R(t)|^2 \rangle$ is given by $u(0, t)$, $u(\rho, t)$ being the solution to (2.5). A method for doing this is shown in the next sections.

We end this section by recalling that in [7] the adjoint equation of (2.5), i.e., the equation for the transition probability density, say p , instead of that above (which, for suitable initial values, furnishes the moments), was solved: An *explicit formula* was obtained for p , and then, by integration against the measure $p \, d\rho$, the moments such as $\langle |R|^2 \rangle$ could be computed. A plot was then obtained by performing such an integration numerically (cf. also [5, 6]).

However, it is highly desirable to solve the PDE above in order to achieve the same results, because this procedure represents a much more general approach, applicable to a wider class of problems where explicit formulae cannot be obtained. Moreover, we want to give a precise extensive tabulation of the values of $\langle |R|^2 \rangle$ and $\langle |T|^2 \rangle \equiv 1 - \langle |R|^2 \rangle$, which does not seem to have been recorded in the existing literature. This is useful in view of several applications of interest at the present time, for instance, in Plasma Physics (cf. [2]).

3. PRELIMINARY CONSIDERATIONS: ABOUT THE SINGULARITIES

We shall solve problem (2.5) by using an implicit scheme of finite differences. However, in order to proceed up to this point, we need to overcome the difficulties that beset Eq. (2.5). In fact, the equation is *degenerate* at $\rho = 1$ (where it is no longer parabolic), and *singular* at $\rho = 0$ (where some coefficient blows up).

As for the degeneracy, we observe that, when $\rho \rightarrow 1^-$, Eq. (2.5) reduces to $u_\tau = 0$, provided that both u_ρ and $u_{\rho\rho}$ remain *bounded*. We can integrate this directly, with the IV $u(\rho, 0) = \rho^2$ (for $\rho = 1$), to get $u(1, t) = u(1, 0) = u(\rho, 0)|_{\rho=1} = 1$.

As for the singularity at $\rho = 0$, by observing that both the PDE and the IV are *even* functions of ρ , we set, by *symmetry*,

$$\left. \frac{\partial u}{\partial \rho} \right|_{\rho=0} = 0 \tag{3.1}$$

(provided only that u_ρ exists up to the boundary $\rho = 0$), which will allow us to dominate the singularity at $\rho = 0$: In the numerical scheme we shall replace

$(u_\rho/\rho)|_{\rho=0}$ with $u_{\rho\rho}|_{\rho=0}$, by l'Hôpital's rule. This idea has been exploited by P. Jamet for handling similar *singularities* in *ordinary* differential equations (cf. [3]).

Therefore, the problem that we solve numerically is

$$\begin{aligned} \frac{\partial u}{\partial \tau} &= (1 - \rho^2)^2 \frac{\partial^2 u}{\partial \rho^2} + \frac{(1 - \rho^2)^2}{\rho} \frac{\partial u}{\partial \rho}, & 0 < \rho < 1, 0 < \tau < T, \\ u(\rho, 0) &= \rho^2, & 0 < \rho < 1 \\ \frac{\partial u}{\partial \rho}(0, \tau) &= 0, & 0 < \tau < T, \\ u(1, \tau) &= 1, \end{aligned} \tag{3.2}$$

where $\tau \equiv (k_0^2/8) I_1 \varepsilon^2 L$, and $T > 0$ is an arbitrary fixed number.

4. NUMERICAL TREATMENT AND DISCUSSION OF THE RESULTS

After the considerations about the singularities in Section 3, we can now implement our scheme of finite differences. We shall use an *implicit* scheme, with forward time-differences and space-centered differences (the Crank–Nicholson scheme; see, e.g., [1, 10]).

We divided the space interval $0 < \rho < 1$ into $N_\rho - 1$ sections of length $\Delta\rho$, and chose a suitable time step-size $\Delta\tau$. We typically chose $N_\rho = 40$ points and $\Delta\tau = 0.04$, so that $\Delta\rho = 1/(N_\rho - 1) \cong 0.0256$ and $\lambda \equiv \Delta\tau/(\Delta\rho)^2 \cong 60.84$.

In order to test convergence, accuracy and stability, however, we varied $\Delta\tau$ and ran the program for $\Delta\tau = 0.016, 0.02, 0.06$ and $N_\rho = 60$, in all possible combinations, also. It turned out that in passing from the value $\Delta\tau = 0.04$ to the value $\Delta\tau = 0.02$ [$\Delta\tau = 0.06$], by keeping $N_\rho = 40$ fixed, the results agreed up to $O(10^{-3})$ [up to $O(10^{-2})$], while, by using $N_\rho = 60$ points we found agreement with the "typical" case $N_\rho = 40, \Delta\tau = 0.04$ up to the order $O(10^{-3})$, for the same value of $\Delta\tau$.

Comparison of the cases $N_\rho = 60$ and $\Delta\tau = 0.02, 0.06$ with the corresponding results for $N_\rho = 40$, showed agreement, respectively, up to $O(10^{-4}), O(10^{-3})$. Comparing, finally, the results obtained for $N_\rho = 60$ by further reducing $\Delta\tau$ from 0.02 to 0.016 showed a variation within the order $O(10^{-3})$.

The accuracy that could be expected theoretically is $O((\Delta\rho)^2) + O((\Delta\tau)^2) \cong O(10^{-3})$ for $\Delta\rho \cong 0.0256$ (corresponding to $N_\rho = 40$) and $\Delta\tau = 0.04$, for the Crank–Nicholson scheme. However, this is correct, strictly speaking, only for the heat equation (cf. [1; 10, p. 189]).

We assumed therefore that good convergence and an accuracy sufficient for our purposes were achieved with $N_\rho = 40, \Delta\tau = 0.04$.

As for the stability, we did not observe any oscillation in any of the cases reported above: Handling the singularity at $\rho = 0$ by means of (3.1) above was essential and no problem arose. The scheme being implicit, we can expect stability for *any* value of λ ; however, the accuracy improves when a *smaller* λ is chosen. The smallest value of λ we used was $\lambda \cong 24.336$, obtained for $N_\rho = 40, \Delta\tau = 0.016$.

The results obtained for $\langle |R(\tau)|^e \rangle \equiv u(0, \tau)$ with the typical values $N_p = 40$, $\Delta\tau = 0.04$ are given in Table I. They seem to be in excellent agreement with the values plotted in [7], which were computed by a numerical quadrature in an explicit formula (see also [5, 6]).

TABLE I
 $\langle |R|^2 \rangle \equiv u(0, \tau)$ versus $\tau \equiv (k_0^2/8) I_1 \varepsilon^2 L$, I_1 Defined in (2.5')

τ	$\langle R ^2 \rangle$	τ	$\langle R ^2 \rangle$
0.04	0.139	1.64	0.965
0.08	0.247	1.68	0.967
0.12	0.334	1.72	0.969
0.16	0.406	1.76	0.971
0.20	0.467	1.80	0.973
0.24	0.520	1.84	0.975
0.28	0.565	1.88	0.976
0.32	0.605	1.92	0.978
0.36	0.639	1.96	0.979
0.40	0.670	2.00	0.980
0.44	0.698	2.04	0.982
0.48	0.723	2.08	0.983
0.52	0.745	2.12	0.984
0.56	0.765	2.16	0.985
0.60	0.783	2.20	0.986
0.64	0.799	2.24	0.987
0.68	0.814	2.28	0.987
0.72	0.828	2.32	0.988
0.76	0.840	2.36	0.989
0.80	0.852	2.40	0.990
0.84	0.862	2.44	0.990
0.88	0.872	2.48	0.991
0.92	0.881	2.52	0.991
0.96	0.889	2.56	0.992
1.00	0.897	2.60	0.992
1.04	0.904	2.64	0.993
1.08	0.910	2.68	0.993
1.12	0.916	2.72	0.994
1.16	0.922	2.76	0.994
1.20	0.927	2.80	0.994
1.24	0.932	2.84	0.995
1.28	0.936	2.88	0.995
1.32	0.940	2.92	0.995
1.36	0.944	2.96	0.996
1.40	0.948	3.00	0.996
1.44	0.951	3.04	0.996
1.48	0.954	3.08	0.996
1.52	0.957	3.12	0.996
1.56	0.960	3.16	0.997
1.60	0.962	3.20	0.997

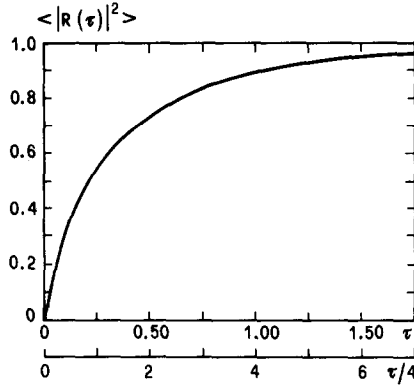


FIG. 1. $\langle |R(\tau)|^2 \rangle \equiv u(0, \tau)$ plotted versus $\tau \equiv (k_0^2/8) I_1 \varepsilon^2 L$, I_1 being defined in (2.5'). Note that in Ref. [7] the abscissa is, instead, $4\tau = (k_0^2/2) I_1 \varepsilon^2 L$.

In Fig. 1 we plotted, for convenience, $\langle |R(\tau)|^2 \rangle \equiv u(0, \tau)$ (cf. the graph of $\langle |T(\tau)|^2 \rangle = 1 - \langle |R(\tau)|^2 \rangle$ in [2, 5, 7]). Here we give a proof of the *monotonicity* of such a quantity as a function of τ ($\tau \propto \varepsilon^2 L$), of which there is numerical evidence, besides physical justification. This is much easier if we start from the PDE (2.5) rather than using the *explicit* formula given in [7].

As the PDE in (2.5), (3.2) has coefficients independent of τ , the quantity $v(\rho, \tau) \equiv u_\tau(\rho, \tau)$ solves the same equation:

$$\frac{\partial v}{\partial \tau} = (1 - \rho^2)^2 \frac{\partial^2 v}{\partial \rho^2} + \frac{(1 - \rho^2)^2}{\rho} \frac{\partial v}{\partial \rho}, \quad 0 < \rho < 1, \tau > 0. \tag{4.1}$$

Moreover, by using (2.5) and the initial value, $u(\rho, 0) = \rho^2$, we obtain

$$\begin{aligned} v(\rho, 0) \equiv u_\tau(\rho, 0) &= (1 - \rho^2)^2 \frac{\partial^2 u(\rho, 0)}{\partial \rho^2} + \frac{(1 - \rho^2)^2}{\rho} \frac{\partial u(\rho, 0)}{\partial \rho} \\ &= 4(1 - \rho^2)^2 \geq 0, \quad \text{for } 0 \leq \rho \leq 1. \end{aligned} \tag{4.2}$$

As

$$\left. \frac{\partial v}{\partial \rho} \right|_{\tau=0} \equiv \left. \frac{\partial u_\tau}{\partial \rho} \right|_{\tau=0} = \frac{\partial}{\partial \tau} [u_\tau(0, \tau)] = 0 \tag{4.3}$$

(true also because of the symmetry) and

$$v(1, \tau) \equiv u_\tau(1, \tau) = \frac{\partial}{\partial \tau} u(1, \tau) = 0 \tag{4.4}$$

(cf. (3.2)), it follows from the maximum principle that

$$0 \leq v(\rho, \tau) \leq 4, \tag{4.5}$$

i.e., in particular, $u_i(\bar{\rho}, \tau) \geq 0$ for every $\bar{\rho}$ with $0 \leq \bar{\rho} \leq 1$. This shows, for $\rho = 0$, the monotonicity above. Moreover, it results from (3.2) and the maximum principle that $0 \leq u(\rho, \tau) \leq 1$, so that, in particular, $0 \leq \langle |R(\tau)|^2 \rangle \leq 1$ follows.

Finally, we studied the rate of approach of the solution of (3.2) to the *stationary value* $u(\rho, \infty) \equiv 1$. In Figs. 2 and 3 we plotted $u(\rho, \tau_j)$ versus ρ for $0 \leq \rho \leq 1$, for several values of $\tau = \tau_j$, j representing the time-steps number. Such a rate could be estimated by

$$\max_{0 \leq \rho \leq 1} \frac{u(\rho, \tau_{j+10})}{u(\rho, \tau_j)}, \quad (4.6)$$

for various j . This quantity must approach 1, when τ_j gets large. Regarding the main quantity of interest, $\langle |R(\tau)|^2 \rangle \equiv u(0, \tau)$, we can just compute the ratio

$$r_j \equiv \frac{u(0, \tau_{j+10})}{u(0, \tau_j)}, \quad (4.7)$$

for which we get $r_{40} \cong 0.980/0.962 \cong 1.0187$, $r_{50} \cong 0.990/0.980 \cong 1.0102$, $r_{60} \cong 0.994/0.990 \cong 1.0040$ (cf. Table I and Figs. 2 and 3), and $r_{70} \cong 0.997/0.994 \cong 1.0030$ (cf. Table I).

The parameters in (4.6), (4.7) give the rate of approach of the solution to its steady-state by relating the values of u to the *number* of time steps (of size

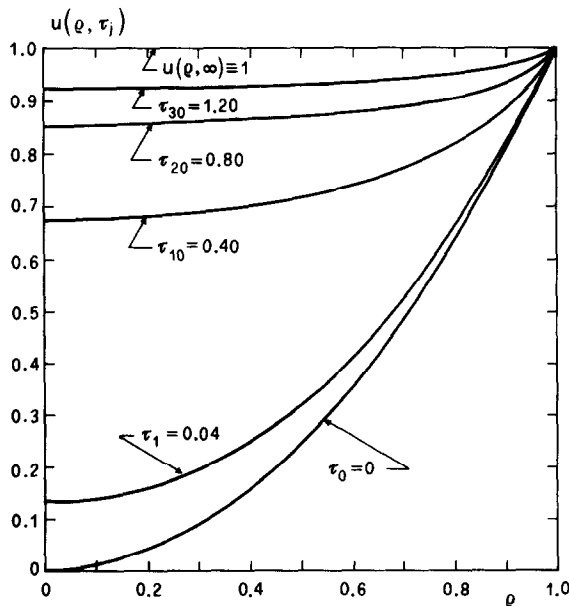


FIG. 2. $u(\rho, \tau_j)$ versus ρ for several values of τ_j , corresponding to 1, 10, 20, 30 time steps.

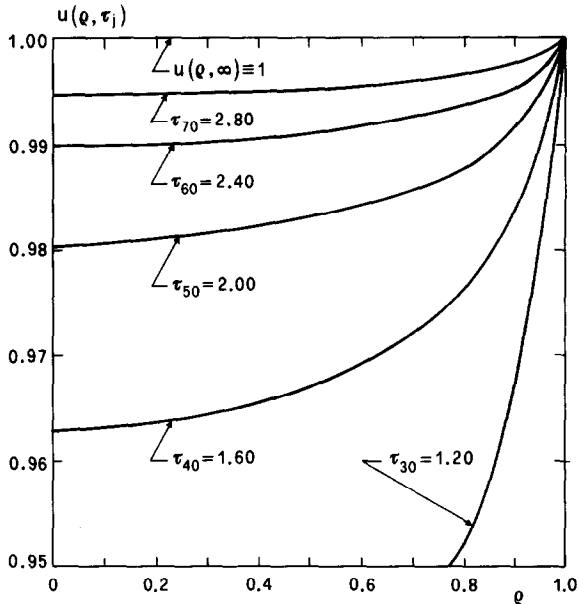


FIG. 3. $u(\rho, \tau_j)$ versus ρ for several values of τ_j , corresponding to 40, 50, 60, 70 time steps.

$\Delta\tau = 0.04$). We can measure such a rate of approach relating the relative variation of u to τ , by the ratio

$$s_j \equiv \left| \frac{\Delta u_j}{u_j \Delta \tau_j} \right| \equiv \left| \frac{u(\rho, \tau_{j+10}) - u(\rho, \tau_j)}{u(\rho, \tau_j) \Delta \tau_j} \right| = \frac{1}{\Delta \tau_j} \left| \frac{u(\rho, \tau_{j+10})}{u(\rho, \tau_j)} - 1 \right|, \quad (4.8)$$

where $\Delta \tau_j \equiv \tau_{j+10} - \tau_j = 10 \Delta \tau = 0.4$. We obtain, for $\rho \cong 0$: $s_{40} \cong 0.0187/0.4 \cong 0.046$, and similarly $s_{50} \cong 0.0102/0.4 \cong 0.025$, $s_{60} \cong 0.0040/0.4 = 0.010$, $s_{70} \cong 0.0030/0.4 \cong 0.007$.

5. SUMMARY

The problem of solving numerically a certain parabolic equation which is singular at certain points of the boundary, has been worked out in detail. The effect of the singularities has been investigated and dominated in a suitable way. Then, a finite-difference scheme has been implemented to compute the solution. Finally, we have discussed the results as well as the accuracy and stability of the method. A table of values of the physically relevant quantity, the mean power reflected by a random medium, has been provided within the order $O(10^{-3})$. The monotonic character of such a quantity as a function of $\varepsilon^2 L$, ε being the "size of the noise" and L the width of the slab of the random medium, which is evident from the numerical

results, have been proved. Some graphs which show the speed of approach of the solution to its stationary value have also been given.

All the computations were carried out on the CDC/Cyber 170, at the Courant Institute of Mathematical Sciences, New York University.

APPENDIX

One can show that, under suitable but rather general hypotheses, the stochastic process solution to the stochastic differential equation

$$\begin{aligned} y'(x) &= \varepsilon F(x, y(x), z(x)), & y(x) \in \mathbb{R}^n, z(x) \in \mathbb{R}^m \\ y(0) &= y, \end{aligned} \tag{A1}$$

where ε is a small parameter, $z(x)$ is a suitable stochastic process, $E\{F\} = 0$, $E\{\cdot\}$ denoting expected values, converges in some sense to a limiting stochastic process, say y^0 (cf. [4; 8, pp. 26–27], see also [9, pp. 540–541], when $\varepsilon \rightarrow 0$, $x \rightarrow \infty$, with $\varepsilon^2 x$ fixed. Such a process turns out to be a *diffusion* process and its statistics can thus be described by the relevant Fokker–Planck equation or, alternatively, by the corresponding Kolmogorov backward equation. The latter has the form

$$u_t = L[u] \quad (t \equiv \varepsilon^2 x), \tag{A2}$$

with

$$L \equiv \sum_{i,j=1}^n a_{ij}(y) \frac{\partial^2}{\partial y_i \partial y_j} + \sum_{i=1}^n b_i(y) \frac{\partial}{\partial y_i}, \tag{A3}$$

where a_{ij} , b_i can be evaluated from F . We can compute the *conditional expectation* of any bounded continuous functional of y^0 , $f(y^0(t))$, by solving (A2) with the *initial value*

$$u(y, 0) = f(y), \tag{A4}$$

getting

$$E_{y,z}\{f(y^0(t))\} = u(0, t), \tag{A5}$$

(cf., e.g., [8, pp. 26–27] or [9, p. 541]). For example, we can compute the second moment $E_{y,z}\{|y^0(t)|^2\}$, by solving (A2) with the initial value $f(y) = |y|^2$. We can then consider this as an approximation for the corresponding quantity for $y(x)$, the solution to (A1), when ε is sufficiently small and x is sufficiently large.

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