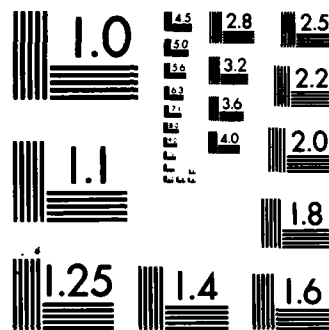


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G C PAPANICOLAOU 31 OCT 83 AFOSR-TR-84-0290
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Annual Report on Grant AFOSR-80-0228

George C. Papanicolaou, Principal Investigator

Period August 1, 1982 - October 31, 1983

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During this period the following scientists and students were supported, in addition to the principal investigator:

G. Beylkin Post-Doctoral Scientist
K. Golden Graduate Student
B. LeMesurier Graduate Student

The following papers have appeared, have been submitted for publication, or are in the final stages of preparation:

- K. Golden and G. Papanicolaou. Bounds for effective parameters of heterogeneous media by analytic continuation. Comm. Math. Phys. 90 (1983), pp. 473-491.
- G. Beylkin. Gaussian beams and representation of the Green's function. Submitted to Wave Motion.
- D. McLaughlin, G. Papanicolaou and O. Pironneau. Convection of Microstructure. Submitted to SIAM J. on Applied Mathematics.
- G. Papanicolaou. Diffusions and random walks in random media. In Mathematics and Physics of Disordered Media, Springer Lecture Notes in Mathematics #1035, 1983.
- R. Figari, E. Orlandi and G. Papanicolaou. Diffusive behavior of a random walk in a random medium. Proceedings of Kyoto Conference, 1982, N. Ikeda, editor, to appear.
- G. Papanicolaou. Macroscopic properties of composites, bubbly fluids, suspensions and related problems. Eyrolles, France, 1984, to appear. (These are the lecture notes for a series of 13 lectures given in July 1983.)
- D. Dawson and G. Papanicolaou. Random wave processes. In preparation.

Remarks on the research effort

Beylkin, who is now permanently at Schlumberger-Doll Research, Ridgefield, Conn., worked on the use of Gaussian beams to represent wave fields at high frequencies in a manner that is insensitive to singularities such as caustics. Several investigators have been interested in this subject recently (at Exxon in Houston and in New Jersey, at Schlumberger and elsewhere), although there is no clear consensus yet regarding the usefulness of beams relative to more conventional geometrical optics methods. One of

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FIELD	GROUP	SUB. GR.			
19. ABSTRACT (Continue on reverse if necessary and identify by block number) During this period the four investigators (two are graduate students) produced five papers and two lecture note series. Titles include, "Bounds for effective parameters of heterogeneous media by analytic continuation," "Gaussian beams and representation of the Greens function," "Convection of microstructure," "Diffusive behavior of a random walk in a random medium," "Random wave processes," and two lecture note series, "Diffusions and random walks in random media," and "Macroscopic properties of composites, bubbly fluids, suspensions, and related problems." Work continues on algorithm design for and numerical study of the focussing singularity in nonlinear beams. Work also continues on the modeling of flows with microstructure. This report summarizes progress in these areas during the inclusive dates.					
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the principal objectives of Beylkin was to find how the beam representation could help in the analysis of random media. The presence of singularities is a very serious limiting factor there (recent work of B. White at Exxon has analyzed wave fields at high frequency in a random medium up to the onset of caustic formation).

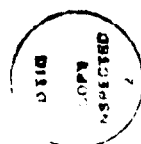
Papanicolaou and Golden continued their work on the analytic continuation method. Golden is writing his dissertation now and will obtain his degree in June 1984. A complete description of progress in this area will be given later. The enclosed paper gives an idea of what had been accomplished until last February.

B. LeMesurier has been working on the focusing singularity for the nonlinear Schrodinger equation, exclusively by numerical computations up to now. The analysis of the focusing singularity is our principal concern now. We want to develop accurate and well structured computational schemes for analyzing singularities in nonlinear beams. As our analytical work has shown (with Weinstein and McLaughlin last year; the final write-up on this is still in preparation), the focusing singularity requires deep and difficult analysis for its solution. It is also a basic problem that arises in many applications in nonlinear wave propagation.

Some work on random media is reported in the enclosed papers. This is work that was done earlier and is continuing at a much reduced pace now.

The works with Dawson and with McLaughlin and Pironneau were discussed earlier. The paper with McLaughlin and Pironneau is included. We want to do much more numerical work in connection with this problem and we will move in this direction in the near future. The paper with Dawson is in preparation. (A copy of the preliminary version was sent earlier.)

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A SUMMARY OF WORK THIS SUMMER ON THE NON-LINEAR SCHRÖDINGER EQUATION

B. LeMesurier

The equation is

$$iu_t + \Delta u + |u|^2 u = 0 \quad \text{on} \quad [0, 2\pi]^2$$

with periodic boundary conditions.

The work done was almost entirely numerical, although some attempts were made to extend results from the case of u in Schwartz class on $\mathbb{R}^2$.

Some previous work of this nature has been done by P.L. Sulem, Cl Sulem and A. Patera [1], giving at least one example of initial data that seems to evolve to "blow up," that is $\sup |u| \rightarrow \infty$ in finite time. I have used their algorithm, as follows

Writing $u_{j,k}^n$ $-M \leq j,k \leq M-1$ for the complex Fourier components of u values on a grid $2M \times 2M$ at time step n , the partially implicit scheme

$$\frac{i(u^{n+1} - u^n)}{\Delta t} + \frac{1}{2}(\Delta u^{n+1} + \Delta u^n) + \frac{3}{2}|u^n|^2 u^n - \frac{1}{2}|u^{n-1}|^2 u^{n-1} = 0$$

gives the Fourier transformed equation

$$\frac{2i}{\Delta t} (\hat{u}_{j,k}^{n+1} - \hat{u}_{j,k}^n) - (j^2 + k^2) (\hat{u}_{j,k}^{n+1} + \hat{u}_{j,k}^n) + 3 \overbrace{(|u^n|^2 u^n)}_{j,k} - \overbrace{(|u^{n-1}|^2 u^{n-1})}_{j,k} = 0$$

I have worked with M a power of two, usually 32, to allow greatest speed in computation of Fast Fourier Transforms.

Algorithms were written for these as this turned out to be faster than the available packaged code (N.C.A.R.) for general M .

Input Parameters

In addition to an array of initial values for u , there are

dt	the time step size
ttime	the maximum time to which solution will be continued
umax	a maximum value for $\max u$

The solver stops when either the ttime or umax limit is attained.

IPF	graphics output is generated every IPF time-steps
ISF	printed output as specified below is generated every ISF time-steps

Typically ISF << IPF

Output

The graphics output currently consists of an array of values of $|u|$, with boundary values repeated at both boundaries. This is input to contour plotting and other programs.

The current time is also output. (Other graphics output, in particular phase information, is now being added.)

The printed data consists of a list of the above input parameters, and the following (Additions are frequently made to this list as new questions arise)

$$\left. \begin{aligned} E &= \int |u|^2 \\ H &= \int (|\nabla u|^2 - \frac{1}{2}|u|^4) \end{aligned} \right\} *$$

These are conserved by the P.D.E. but not the algorithm, so measure accuracy of the solver.

$$\left. \begin{aligned} \max |u| \\ \int |\nabla u|^2 \\ \int |u|^4 \end{aligned} \right\} \text{ These three should all "blow-up" for suitable initial data.}$$

The remaining quantities are "localized"; the integrals are taken over a disc in the center of the period. This part of the output was added after summer, principally to study the variance of part of the data, which in the Schwartz class data case is the key to proving blow-up.

Thus a new input parameter RL is added, and
 $B = \{(x,y) : |x-\pi|^2 + |y-\pi|^2 \leq (2\pi RL)^2\}$ in the following list of output quantities

$$v_{loc} = \int_B |u|^2 r^2 \quad r^2 + |x-\pi|^2 + |y-\pi|^2,$$

* Various factors of $4\pi^2$ etc. are omitted.

Backward difference estimates of

$$\frac{d}{dt} v_{loc} \quad \text{and} \quad \frac{d^2}{dt^2} v_{loc} ,$$

$$E_{loc} = \int_B |u|^2 ,$$

$$H_{loc} = \int_B |\nabla u|^2 - \frac{1}{2} |u|^4 ,$$

$$\int_B |\nabla u|^2 ,$$

$$\int_B |u|^4 .$$

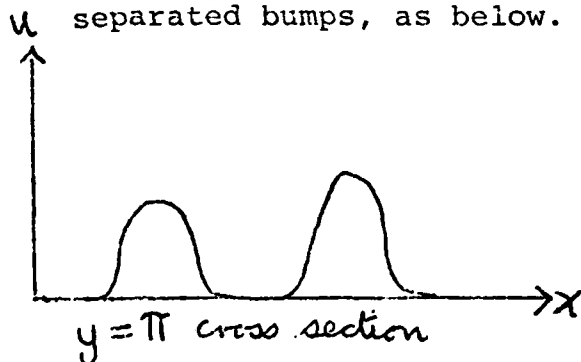
Observations

Initial data has mostly been chosen with a "bump" shape: one or two maxima near the period's center, dying off to small values (and small gradients) near the boundary. All have been real valued, and most have had $H < 0$, a condition guaranteeing blowup in the Schwartz class (i.e. all space) case.

The results has been, consistently, growing and narrowing of the bump at an accelerating rate, as expected from the all space case. However limitations on resolution only allow a growth in $\max|u|$ by a factor of about 3 before computational errors become substantial: a finer grid will be needed in later work.

As one hope is that the evolution of a bump to blow-up is mostly local (not affected much by values away from the bump so long as they are small or flat, say) experiments have been done where the central bump is left unchanged, but the values outside are set to various different constants (smoothly connected to the bump).

The results are promising: the rate and nature of the blow-up changes little, and the near-constant outer region evolves much as if the bump were not present. That is, it retains constancy in space and the same absolute value, to a fair degree. A second localization test was the use of two separated bumps, as below.



The evolution was compared to the evolution of data with just one or the other bump.

Again the results were pleasing: the two bumps seem to evolve in ignorance of each other.

Later work (after the summer) has studied the localized variance of a bump, as mentioned above. The motivation is the result

$$\frac{d^2 V}{dt^2} = 8H, \quad V = \int |u(x,t)|^2 |x|^2 dx \quad \text{for the all-space case.}$$

Local variances have been studied with the cutoff well down the shoulder of a bump, with and without radial symmetry, and with the value outside the cutoff not necessarily going to zero. (The value near the boundary has always been a constant, initially.)

The local variance has consistently evolved with

$$\frac{d^2}{dt^2} V_{loc} / H_{loc} \approx 8 .$$

In the case of localization containing the support of the initial data, the ratio seems to be a little less. This is reasonable as $u(x,0) = C$, a constant gives $V_{loc} = \text{constant}$, $H < 0$.

As yet, V_{loc} has not got near 0 in the runs, and it is not clear whether or not it would approach close to 0 before blow-up occurs. This question awaits higher resolution computations.

- [1] P. L. Sulem, C. Sulem and A. Patera, "Numerical Simulation of Singular Solutions to the Two-dimensional Cubic Schrödinger Equation." In the thesis of C. Sulem, L'Université Paris-Nord.

1. The Analytic Continuation Method for Two-Component Media

Let (Ω, F, P) be a probability space and $\epsilon(x, \omega)$ be a stationary random field on $x \in \mathbb{R}^d$ and $\omega \in \Omega$. For two-component media let $\epsilon(\omega) = \epsilon_1 \chi_1(\omega) + \epsilon_2 \chi_2(\omega)$ be the dielectric constant at the origin in $\mathbb{R}^d$ of the realization $\omega \in \Omega$ of the material, where $\chi_1 = 1$ if medium 1 occupies the origin and $\chi_1 = 0$ otherwise, similarly for χ_2 . The effective dielectric constant of the composite may be defined as

$$\epsilon^* = \int_{\Omega} P(d\omega) \epsilon(\omega) \vec{E}(\omega) \cdot \vec{e}_k, \quad (1)$$

where $\vec{E}$ is the electric field at the origin with average $\vec{e}_k$, a unit vector in the k^{th} direction. It is useful to consider the function $F(s) = 1 - m(h)$ where $m(h) = \epsilon^* / \epsilon_2 (\epsilon_1 / \epsilon_2)$ and $s = 1/(1-h)$. Maxwell's equations yield a resolvent expression for $\vec{E}$ so that

$$F(s) = \int_{\Omega} P(d\omega) \chi_1 (s + \Gamma \chi_1)^{-1} \vec{e}_k \cdot \vec{e}_k \quad (2)$$

where $\Gamma = \nabla(-\Delta)^{-1} \nabla$. The spectral theorem in an appropriate Hilbert space then gives

$$F(s) = \int_0^1 \frac{d\mu(z)}{s - z}, \quad (3)$$

where μ is the positive Borel measure on $[0,1)$ arising from the family of projections associated with the self adjoint operator $\Gamma \chi_1$. The representation (3) can also be proved by noting that $\text{Im}(-F) > 0$ when $\text{Im}(s) > 0$ and that F is analytic off $[0,1]$ with $F(\infty) = 0$. Then a general theorem in function theory gives (3).

For $|s| > 1$ we can expand (2) about a homogeneous medium ($h=1$ or $s=\infty$),

$$F(s) = \int_{\Omega} P(d\omega) \left[\frac{\chi_1}{s} - \frac{\chi_1 \Gamma_{kk} \chi_1}{s^2} + \frac{\chi_1 \Gamma_{kk} \chi_1 \Gamma_{kk} \chi_1}{s^3} - \dots \right], \quad (4)$$

where $\Gamma_{kk} = \frac{\partial}{\partial x_k} (-\Delta)^{-1} \frac{\partial}{\partial x_k}$. Equating (4) to the $\frac{1}{s}$ expansion of (3)

determines the moments of μ . Then (3) provides the analytic continuation of (4) from $|s| > 1$ to the full domain of analyticity of $F(s)$. If (4) is assumed known only to first order, then only the mass p_1 of μ is fixed, where p_1 is the volume fraction of medium 1. Under this assumption we obtain for fixed $s \notin [0,1)$ extremal values of the linear functional $F_s(\mu)$ by evaluating (3) with Dirac point masses, since they are the extreme points of the set of positive Borel measures on $[0,1)$ with fixed mass. The resulting bounds restrict $F_s(\mu)$ to a region in the complex plane bounded by two circular arcs, which give for real s the classical Wiener bounds $(p_1/\epsilon_1 + p_2/\epsilon_2)^{-1} \leq \epsilon^* \leq p_1\epsilon_1 + p_2\epsilon_2$. If the material is further assumed to be statistically isotropic, then it is possible to calculate the second term in (4). This F known to second order can be transformed to a function of the type (3) known only to first order, the extremization of which gives the Hashin-Shtrikman bounds, which were first found using a variational principle. The transformation procedure works to any order in (4).

2. Extension to Multicomponent Media

As Bergman [6] and Milton [7] point out, it is not clear from the two-component case how to extend the analytic method to three or more components. We now describe such an extension. For simplicity we consider only three-component materials. The effective parameter ϵ^* is then an analytic function of two complex variables $h_1 = \epsilon_1/\epsilon_3$ and $h_2 = \epsilon_2/\epsilon_3$ with $\text{Im } \epsilon^* > 0$ on $\{\text{Im } h_1 > 0\} \times \{\text{Im } h_2 > 0\}$. The key step in the extension is to obtain a representation formula analogous to (3). Using Cauchy's theorem in several variables we have proven the following for the polydisc $D^2 = \{|z_1| < 1\} \times \{|z_2| < 1\}$: for $f(z_1, z_2)$ to be analytic with non-negative real part in D^2 it is necessary and sufficient that f may be represented as

$$f(z_1, z_2) = iv(0,0) + \frac{1}{2} \int \int_{T^2} (H_1 H_2 + H_1 + H_2 - 1) d\mu(t_1, t_2), \quad (5)$$

where $H_j = (e^{it_j + \zeta_j}) / (e^{it_j - \zeta_j})$, $j = 1, 2$, $v = \text{Im} f$, and $u \in M_q$,

$$M_q = \left\{ \begin{array}{l} \text{positive Borel measures of mass } q \text{ on the torus } T^2 \\ \text{satisfying the condition } \int \int_{T^2} e^{i(nt_1 + mt_2)} d\mu(t_1, t_2) = 0 \\ \text{when } nm < 0 \end{array} \right\}. \quad (6)$$

We evaluate (5) with $d\mu(t_1, t_2) = dv_1(t_1) \times dt_2 + dt_1 \times dv_2(t_2)$, where v_1 and v_2 are positive measures on the circle. Let $U^2 = \{\operatorname{Im} s_1 > 0\} \times \{\operatorname{Im} s_2 > 0\}$, where each factor U is conformally equivalent to the disc D , with $s_1 = 1/(1-h_1)$ and $s_2 = 1/(1-h_2)$. Now, a function $K(s_1, s_2)$ analytic on $U^2 \cup \bar{U}^2 \cup (([0,1] \times \mathbb{R}) \cup (\mathbb{R} \times [0,1]))^c$ with $\operatorname{Im} K > 0$ on U^2 and $K(\infty, \infty) = 0$, where "-" denotes complex conjugation and "c" denotes complementation in $\mathbb{R}^2$, has the representation

$$K(s_1, s_2) = \int_0^1 \frac{d\mu_1(z_1)}{z_1 - s_1} + \int_0^1 \frac{d\mu_2(z_2)}{z_2 - s_2}, \quad (7)$$

where μ_1 and μ_2 are positive measures arising from v_1 and v_2 . If $K(s_1, s_2) = -F(s_1, s_2)$ then the expansion of $F(s_1, s_2)$ corresponding to (4) forces the masses of μ_1 and μ_2 to be p_1 and p_2 , the volume fractions of media 1 and 2, respectively. If μ_1 and μ_2 are point masses at $z_1 = z_2 = 0$ then μ on the torus is an extreme point of $M_{p_1+p_2}$. Such μ give

the real Wiener bounds. When the material is statistically isotropic F has a non-zero second order crossterm in its expansion, so that (7) is not applicable.

However, the function $G = F / (1 - \frac{1}{d} F)$ has the expansion

$$G(s_1, s_2) = \frac{p_1}{s_1} + \frac{p_2}{s_2} + \frac{p_1}{ds_1^2} + \frac{p_2}{ds_2^2} + \frac{0}{s_1 s_2} + \dots. \text{ Letting } K = -G \text{ with } \mu_1 \text{ and } \mu_2$$

point masses at $z_1 = z_2 = 1/d$ gives the real Hashin-Shtrikman bounds for three-component materials.

Currently we are working on proving for the first time complex versions of the Wiener and Hashin-Shtrikman bounds for three-component materials which restrict F to regions bounded by circular arcs. In our formalism, establishing these bounds and the previous real ones depends on showing that for fixed $(\zeta_1, \zeta_2) \in D^2$, the extremal values of the linear functional $f_{\zeta_1, \zeta_2}(\mu)$ on M_1 are attained when $d\mu = \delta_{t_1^*} \times dt_2$ or $d\mu = dt_1 \times \delta_{t_2^*}$, where $t_1^*, t_2^* \in [0, 2\pi)$.

We have evidence that such a statement is true and are working to prove it. These matters will be contained in the author's Ph.D. thesis.

Underlying a full understanding of the three-component problem is the characterization of the set of extreme points of M_1 . Rudin [5] and McDonald [8] have given examples of these extreme points but a full characterization of them is still unknown. It is not even known if all the extreme points are singular with respect to the Haar measure on T^2 . We propose to analyze the extremal structure of M_1 . One way of gaining insight is to consider the set

of positive measures $M_1^{n \times n}$ satisfying the Fourier condition in (6) living not on T^2 , but on a discrete model of T^2 , namely $T_{n \times n}^2 = \{\omega^0, \omega^1, \dots, \omega^{n-1}\} \times$

$\times \{\omega^0, \omega^1, \dots, \omega^{n-1}\}$, $\omega = e^{i2\pi/n}$. For a measure $d\mu = \sum_{i,j=0}^{n-1} \alpha_{ij} \delta_{\omega^i, \omega^j}$ on

$T_{n \times n}^2$, condition (6) gives $(n-1)^2 + 1$ equations in the n^2 unknowns α_{ij} .

We have an algorithm which enumerates all the extreme points of $M_1^{n \times n}$, which is a convex compact subset of $\mathbb{R}^{n^2 - (n-1)^2 - 1}$. Hopefully, analysis of $M_1^{n \times n}$ will shed some light on the structure of M_1 . We should also mention that McDonald [8] has established an isomorphism between M_1 and a certain family Q of linear operators on the disc algebra. Analyzing the extreme points of Q should give information about those of M_1 .

In [4] we rederive the classical Hashin-Shtrikman bounds for three-component materials using analytic continuation. Milton [7] has shown that for certain volume fraction regimes these bounds are not optimal, i.e. there does not exist a material that attains them. He conjectures tighter "bounds," but as yet they remain unproved. We hope to settle this question using the methods

we have developed. One approach is to understand more fully the fractional linear transformations of $F(s_1, s_2)$ that we use to derive bounds on ε^* , in the hope of finding one that might yield better bounds for certain volume fractions. Since certain transformations of F induce a nonlinear mapping from M_q into M_q , a related approach is to look for extreme points different from the ones used in the beginning of this section that would perhaps give better bounds for certain volume fractions.

Finally, in section 1 we alluded to a procedure which gives bounds incorporating n^{th} order information in (4). We hope to do the same for multi-component media by using fractional linear transformations.

3. Application to the Conductivity Problem in Bond Percolation

If the heterogeneous "material" is a square lattice composed of bonds of conductivity σ_1 with probability p_1 and σ_2 with probability $p_2 = 1 - p_1$, then at percolation ($h = \sigma_1/\sigma_2 = 0$ or $s = 1$) the expansion of (3) gives

$$F(1) = \mu^{(0)}(p_1) + \mu^{(1)}(p_1) + \mu^{(2)}(p_1) + \dots, \quad (8)$$

where $F = 1 - \sigma^*/\sigma_2$, σ^* is the effective conductivity of the lattice and the $\mu^{(n)}$ are the moments of μ . Expansion (4) gives

$$\mu^{(n)} = (-1)^n \int_{\Omega} P(d\omega) \chi_1((\Gamma \chi_1)^{n\rightarrow} \vec{e}_k) \cdot \vec{e}_k. \quad (9)$$

Bergman and Kantor [9] realized that since the bonds are independent, the moments $\mu^{(n)}$ can be calculated in terms of polynomials in p_1 with coefficients composed of infinite series involving the lattice Green's function $g(x, y)$ with $x, y \in \mathbb{Z}^d$. Independently, we computed the first four moments of μ with

$$\mu^{(0)} = p_1, \quad \mu^{(1)} = p_1 p_2 / d \quad \text{and} \quad \mu^{(2)} = \left(\sum_{j=1}^d (D_k^+ D_j^- g(0, 0))^2 \right) A_3(p_1) - (D_k^+ D_k^- g(0, 0)) p_1 A_2(p_1),$$

where $D_k^+ D_j^-$ denotes the k, j second difference, and

$$A_N(p_1) = (-p_1)^N + \sum_{k=1}^N \binom{N}{k} (-1)^{N-k} p_1^{N-k+1}.$$

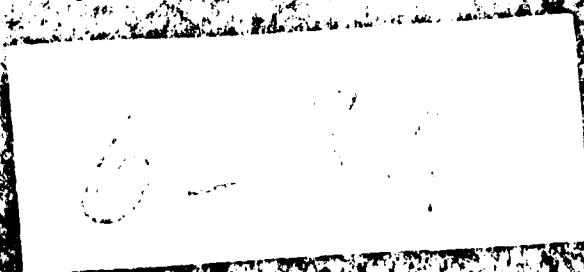
The fourth moment involves one of the above-mentioned infinite series. Note that for $d=2$ the Keller relation $m(h)m(1/h)=1$ determines the odd moments of μ in terms of lower order even moments. While we understand the general structure of the n^{th} moment and could with great patience compute, say, the 20^{th} , we have as yet been unable to write down a general formula for $\mu^{(n)}$. To understand the percolation threshold one must understand the properties of $\mu^{(n)}$ for large n . The hope is that perhaps for $d=2$ we will be able to extract enough information about the $\mu^{(n)}$ to analyze the critical exponent and critical probability. We would like to apply graph theoretic methods to the problem as the expansion (4) is similar to those that arise in quantum field theory and statistical mechanics. Another approach is to use the procedure alluded to at the end of section 1 to obtain tighter bounds on $F(1)$ as more of the moments of μ are known.

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