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Bulk Conductivity of the Square Lattice for Complex Volume Fraction

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Abstract. The bulk conductivity $\sigma^*(p)$ of the bond lattice in $\mathbb{Z}^d$ is considered, where the conductivity of the bonds is 1 with probability p or $\epsilon \geq 0$ with probability $1-p$. The behavior of $\sigma^*(p)$ for complex p is investigated numerically and analytically. We find numerical evidence that the phase transition occurring at the percolation threshold p_c is characterized by a domain "splitting," where $\sigma^*(p) = 0$ in a region containing $(0, p_c]$ while $\sigma^*(p) \neq 0$ in a region containing $(p_c, 1]$. Furthermore, the loss of analyticity at p_c does not appear to arise from a "pinching" of zeros around p_c, as in the Lee-Yang picture of phase transitions. A partition function for σ^* is introduced and is similarly analyzed.

1. Introduction.

Random resistor networks [1-3] based on the percolation model provide an excellent setting in which to study disordered conductors. In particular, we consider the bulk conductivity $\sigma^*(p)$ of the bond lattice in $\mathbb{Z}^d$, where the conductivity of the bonds is either 1 with probability p or $\epsilon \geq 0$ with probability $1-p$. What is particularly interesting about this model is that for $\epsilon = 0$ it exhibits a phase transition at a critical probability $p_c \in (0,1)$, i.e. for $p < p_c, \sigma^*(p) = 0$, while $\sigma^*(p) > 0$ for $p > p_c$. This critical probability p_c coincides [4,5] with the percolation threshold p_c, below which $P_\infty(p) = 0$, where $P_\infty(p)$ is the probability that the origin belongs to an infinite cluster of occupied (conductivity 1) bonds, and above which $P_\infty(p) > 0$. As $p \to p_c^+$, it is believed that $\sigma^*(p)$ exhibits critical scaling, $\sigma^*(p) \sim (p-p_c)^t$, where t is called the conductivity critical exponent.

It is interesting both mathematically and physically to understand the exact nature of the conducting phase transition at p_c. In previous work [6] we proved that for every $\epsilon > 0$, $\sigma^*(p)$ is analytic in an open neighborhood of [0,1] in the complex p-plane. This result establishes that for $\epsilon > 0$, no phase transition can occur. As $\epsilon \to 0$, $\sigma^*(p)$ loses analyticity, at least at $p = p_c$. Analogously, with $\epsilon = 0$, the finite volume version $\sigma_L^*(p)$ of $\sigma^*(p)$, where L is the length of a side of a box of volume L^d, is a polynomial in p, which is an (entire) analytic function of p. As the infinite volume limit is taken,

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analyticity is again lost, at least at $p = p_c$. The question arises as to exactly how this analyticity is lost.

In the Lee-Yang picture of phase transitions [see, e.g., ref. 7], the finite volume partition function is a polynomial in the fugacity, whose zeros lie off the positive real axis, reflecting the absence of a phase transition for finite volumes. As the infinite volume limit is taken, these zeros coalesce into a curve, and "pinch" the real axis, causing a loss of analyticity at the critical fugacity. For certain systems, even for small volumes the zeros lie on a well defined curve.

In this work we investigate $\sigma_L^*(p)$ for complex p in the case of the $d = 2$ square lattice. If the lattice has N bonds, then $\sigma_L^*(p)$ is an N^{th} order polynomial in p. We use the computer to calculate the conductivities of realizations of the random network, which yields the coefficients of the polynomial. Then the program Mathematica is used to obtain various graphs of $\sigma^*(p)$ in the complex p-plane. We have only considered lattices of size up to 9×9, with $\epsilon = 0.001$, but there are certain discernible features of $\sigma^*(p)$ which are common to all the graphs. The principal feature is that there appears to be a region W, which can be very roughly described by

$$W \approx \{\, p \,|\, 0 \leq \mathrm{Re}\; p < p_c, -0.1 < \mathrm{Im}\; p < 0.1 \,\},$$

such that $\sigma^*(p)$ appears to vanish in W. Apparently the domain of analyticity of $\sigma^*(p)$ around [0,1] appears to be split around p_c (although it is not rigorously known that $\sigma^*(p)$ is analytic anywhere). This splitting of the domain (or the splitting of the function into two separate analytic pieces) is part of the Lee-Yang picture, where the line of zeros splits the domain of analyticity of the partition function. However, we have as yet found no evidence of zeros pinching the Re p axis around p_c. In addition to $\sigma_L^*(p)$, we shall define a partition function for the problem, and note that it has a similar behavior to $\sigma_L^*(p)$ for complex p.

2. Formulation.

We formulate the bond conductivity problem for an arbitrary graph. Let G be a finite graph consisting of N bonds $\{b_i\}$ and M vertices $\{x_i\}$. Assigned to G are N independent random variables c_i, $1 \leq i \leq N$, the bond conductivities, which take the values 1 with probability p and $\epsilon \geq 0$ with probability $q = 1 - p$. Distinguish two vertices, say $x_1 = x$ and $x_M = y$, and connect them to a battery which keeps the voltage drop between them equal to 1. The effective conductivity $\widetilde{\sigma}(\omega)$ of the network for any realization ω of the bond conductivities is just the total current $i(\omega)$ that flows through the network, which is obtained via Kirchoff's laws. We define $\sigma(p) = < \widetilde{\sigma}(\omega) >$, where the expectation $< \cdot >$ is over all 2^N realizations. For example, a two bond network has

$$\sigma(p) = p^2 \widetilde{\sigma}(1, 1) + pq(\widetilde{\sigma}(1, \epsilon) + \widetilde{\sigma}(\epsilon, 1)) + q^2 \widetilde{\sigma}(\epsilon, \epsilon) \ ,$$

where $\widetilde{\sigma}(1,1) = \widetilde{\sigma}(\omega)$ with $\omega = (1,1)$, and so on. For N bonds, $\sigma(p)$ is an Nth order homogeneous polynomial in p and q,

$$\begin{aligned} \sigma(p) &= \sum_{k=0}^{N} \alpha_k p^{N-k} q^k \\ \alpha_k &= \sum_{\omega^k \in \Omega^k} \widetilde{\sigma}(\omega^k), \quad q = 1 - p, \end{aligned} \tag{2.1}$$

where $\Omega^k = \{\omega^k = (\omega_1, \ldots, \omega_N) | \omega_\ell = \epsilon$ for exactly k of the ω_ℓ's$\}$.

The cases of most interest are when G is a square, cubic, or hypercubic lattice. Then, with $d = 2$ for simplicity, we take an $L \times L$ sample of the lattice and attach a perfectly conducting bus bar to each of two opposite edges of the sample. This can be accomplished [4] in the above language by attaching to each vertex of these opposing edges a perfectly conducting bond. All of these bonds from one edge meet at a new vertex x and all the bonds from the other edge meet at a new vertex y. Then x and y are connected again with the unit battery. Random bond conductivities are assigned only to the bonds in the original $L \times L$ sample. Let $\sigma_L(p)$ denote (2.1) for the effective conductivity measured between x and y. Then for $d \geq 1$, the finite volume bulk conductivity $\sigma_L^*(p)$ is defined as

$$\sigma_L^*(p) = L^{2-d} \sigma_L(p) \ . \tag{2.2}$$

Finally, we define the bulk conductvity $\sigma^*(p)$ by

$$\sigma^*(p) = \lim_{L \to \infty} \sigma_L^*(p). \tag{2.3}$$

For $\epsilon > 0$, the infinite volume limit in (2.3) has been shown to exist [**8-11**], and for $\epsilon = 0$ the existence of σ^* has recently been proven in the continuum [12].

3. Analyticity for $\epsilon > 0$.

For completeness, we state and prove here the analyticity result which motivates the present investigation. The analysis is based on an integral representation which was proved for two component stationary random media in [**10**] (see also [**13**]). The formulation there is in the continuum, but applies in the present context by replacing the continuum equations for the electric and current fields with their discrete analogs, i.e., Kirchoff's laws. We repeat here only the relevant features.

Let $s = 1/(1-\epsilon)$. We shall consider s to be a complex variable. It can be shown that $\sigma^*(p,s)$ is analytic everywhere in the s-plane except for the interval $[0,1]$. Furthermore, $\sigma^*(p,s)$ maps the upper half plane to the upper half plane, i.e., Im $\sigma^*(p,s) > 0$ when Im $s > 0$. As a consequence of these analytic properties, $\sigma^*(p,s)$ has the following integral representation,

$$1 - \sigma^*(p,s) = \int_0^1 \frac{d\mu(x)}{s - x} \ , \tag{3.1}$$

where μ is a positive Borel measure on $[0,1]$ which depends on p. Notice that this representation separates the dependence of $\sigma^*(p,s)$ on s from its dependence on p. (In fact, (3.1) applies even when $\epsilon = 0$.) The dependence of μ on p is most easily obtained through its moments, as follows. For $|s| > 1$, (3.1) can be expanded about a homogeneous medium ($s = \infty$ or $\epsilon = 1$), yielding

$$1 - \sigma^*(p,s) = \frac{\mu_0(p)}{s} + \frac{\mu_1(p)}{s^2} + \frac{\mu_2(p)}{s^3} + \dots , \tag{3.2}$$

$$\mu_n = \int_0^1 x^n d\mu(x) . \tag{3.3}$$

By equating (3.2) to a similar expansion of a resolvent representation for σ^*, one can obtain a formula for $\mu_n(p)$ in terms of the iterates of a self adjoint operator on L^2 (Ω = set of realizations of the bond conductivities) involving the Green's function of the discrete Laplacian. Because the bond conductivities are independent, these moments can be computed in principle, but they become very complicated. The first two are

$$\begin{aligned} \mu_0(p) &= 1 - p \\ \mu_1(p) &= \frac{p(1-p)}{d} . \end{aligned} \tag{3.4}$$

In general, $\mu_n(p)$ is an $(n+1)$-order polynomial in p.

We are now ready to state

THEOREM 3.1: *($d \geq 1$ bond problem) For every $\epsilon > 0$, there exists an open neighborhood V_ϵ in the complex p-plane such that $[0,1] \subset V_\epsilon$ and $\sigma^*(p)$ is analytic in V_ϵ.*

Proof. Fix $s = 1/(1-\epsilon) > 1$. The idea is to produce a neighborhood containing $[0,1]$ in which (3.2) converges uniformly. Since for $p \in [0,1]$, $\mu_0(p) = 1 - p$ and $\mu_n(p) \geq \mu_{n+1}(p)$ for all n (via (3.3)),

$$\mu_n(p) \leq 1, \quad p \in [0,1] . \tag{3.5}$$

Now we must extend what we can of (3.5) into the complex plane. Consider $E = \{p \in \mathbb{C} | p \notin [0,1]\}$. Conformally map E onto the unit disk D in the z-plane, so that $p = \infty$ gets mapped to $z = 0$, and $[0,1]$ gets mapped to the unit circle $|z| = 1$. Let $m = n + 1$. Since $\mu_n(p)$ is an mth order polynomial in p, $\mu_n(z)$ has at worst an mth order pole at $z = 0$. Thus $z^m \mu_n(z)$ is analytic in D. Since $|\mu_n(z)| \leq 1$ for $|z| = 1$, by the maximum modulus principle,

$$|\mu_n(z)| \leq \frac{1}{|z|^m} , \quad z \in D . \tag{3.6}$$

For any small $\delta' > 0$, there is a small $\delta > \delta' > 0$ such that in the annulus $A_{\delta'}$ defined by $1 \geq |z| > 1 - \delta'$

$$|\mu_n(z)| \leq (1+\delta)^m , \quad z \in A_{\delta'} . \tag{3.7}$$

For our given $s > 1$ (or $\epsilon > 0$), we can choose δ and δ' such that

$$|\mu_n(p)| \leq (1+\delta)^m < s^m , \quad p \in V_\epsilon , \tag{3.8}$$

where V_ϵ conformally maps to $A_{\delta'}$. Then (3.2) converges uniformly in V_ϵ, which proves the theorem.

Remarks. Theorem 3.1 and its proof hold for a large class of continuum systems as well, namely infinitely interchangeable media, which have recently been introduced by O. Bruno [14]. This class is a generalization of Miller's cell materials [15], where all of space is divided up into cells, such as spheres of all sizes, and then the conductivity of each cell is a random variable (independent from the others) taking two (or more) values with probability p and $1-p$. While the integral representation (3.1) holds in great generality, along with (3.5), what is needed to make the proof go through is that the $\mu_n(p)$ are polynomials in p. The proof of this fact for infinitely interchangeable media is contained in [16] (along with rigorous upper and lower bounds on $\sigma^*(p)$ for the $d=2$ bond problem with $\epsilon > 0$). We also note that Theorem 3.1, and its generalization to infinitely interchangeable media, provides a rigorous basis for the volume fraction expansions of $\sigma^*(p)$, which have been widely used for a long time [16]. Finally, Theorem 3.1 presumably does not hold for all composite media. For example, $\sigma^*(p)$ for a periodic array of spheres of volume fraction p embedded in a host material is believed to be analytic at $p=0$ only in the variable $p^{\frac{1}{3}}$, so that $\sigma^*(p)$ has a branch cut there (see, e.g., [17]).

4. Calculation of $\sigma_L^*(p)$.

In order to investigate the behavior of $\sigma_L^*(p)$ for complex p, we numerically calculate the α_k in (2.1), which depend on the effective conductivities of realizations of the lattice with random bond conductivities. It is first useful to describe a beautiful formula which gives the effective conductivity of any graph with any set of conductivities on the bonds.

Let G be a graph with M vertices and N bonds. Without loss of generality we can assume that any two vertices are joined by only one bond, since if there are n bonds joining two vertices, they can be replaced by one bond whose conductivity is the same as the sum of the conductivities of the n bonds. We denote the conductivity of bond b_{ij} joining vertex x_i to vertex x_j by c_{ij}. As in section 2, we distinguish two vertices $x_1 = x$ and $x_M = y$, with $c_{1M} = 0$, and we are interested in the effective conductivity of G (with bond conductivities c_{ij}) measured between vertices x and y, denoted by $\sigma_{xy}(G)$. Our subsequent calculations are based on the following exact formula [18,19], which in some form was known to Kirchoff himself,

$$\sigma_{xy}(G) = \frac{\sum\limits_{T} \prod\limits_{b_{ij}\epsilon T} c_{ij}}{\sum\limits_{T_{xy}} \prod\limits_{b_{ij}\epsilon T_{xy}} c_{ij}} \quad , \tag{4.1}$$

where the sum in the numerator is over all spanning trees in G, and the sum in the denominator is over all spanning trees T_{xy} in G with the vertices x and y identified. Another way of viewing the trees T_{xy} is by considering a new graph G' obtained from G by adding a bond b_{1M} between x and y (the battery bond) with $c_{1M} = h$. The set of trees T_{xy} are then those trees of G' which include b_{1M}, and the denominator of (4.1) is obtained by setting $h = 1$ for those trees.

To implement formula (4.1) on the computer, it is useful to write it in terms of an adjacency matrix [20]. Let the $M \times M$ matrix A be defined by

$$A_{ij} = -c_{ij} \quad , \quad i,j = 1,\dots,M$$
$$A_{ii} = \sum_{j \neq i} c_{ij} \quad , \quad i,j = 1,\dots,M \quad , \tag{4.2}$$

with $c_{1M} = h$. We define two associated matrices as follows. Let A' be the $(M-1) \times (M-1)$ matrix formed from A by removing the first row and first column, corresponding to $x_1 = x$. Then let A'' be the $(M-2) \times (M-2)$ matrix formed from A' by subsequently removing its last row and last column, corresponding in A to $x_M = y$. Finally, define

$$Z(h) = \det(A')$$
$$Z'(h) = \det(A'') \tag{4.3}$$

where "det" means determinant. Then (4.1) can be written as

$$\sigma_{xy}(G) = \left.\frac{\det(A')}{\det(A'')}\right|_{h=0} \tag{4.4}$$

Recalling the statistical mechanics of the Ising model [see also ref. **21**], we can also write (4.4) as

$$[\sigma_{xy}(G)]^{-1} = \frac{Z'(0)}{Z(0)} = \left(\frac{\partial}{\partial h} \ln Z\right)(0) \quad , \tag{4.5}$$

which leads us to think of $Z(h)$ as a partition function, $\ln Z(h)$ as a free energy, and the resistance $[\sigma_{xy}(G)]^{-1}$ as a magnetization. Note that if all the bonds of G have unit conductivity then $Z(0)$ is the number of trees of G.

To calculate $\sigma_L^*(p)$, we let G be the graph described below (2.1), that is, G is an $L \times L$ sample of the $d = 2$ lattice, where L measures the number of vertices on a side. Included in G are the two vertices $x = x_1$ and $y = x_M$, which are attached to the vertices of two opposite sides by perfectly conducting bonds. Then $M = L^2 + 2$, and the number of bonds which have random conductivities 1 or ϵ is $N = 2\big((L-1)^2 + L - 1\big)$. To calculate the α_k in (2.1) we use the following procedure, which was carried out on a Sun 3/60 computer. First, α_0 is just the conductivity of G with the N bonds all assigned the conductivity 1. Then we randomly choose one bond and assign to it the conductivity $\epsilon = 0.001$ (ϵ must not be chosen too close to zero in order to avoid singular matrices), and calculate the resulting conductivity. Of the remaining 1's, we randomly choose another, and continue this procedure until all N bonds have conductivity ϵ. We repeat this procedure 30 times, letting $\overline{\alpha_k}$ be the average conductivity measured when there are k bonds of conductivity ϵ. Then we take

$$\alpha_k = \binom{N}{k} \overline{\alpha_k} \ , \tag{4.6}$$

which yields a reasonable numerical approximation to (2.1). The determinants in (4.4) are calculated by an IMSL routine. Plots of $\sigma_L^*(p)$ for complex p are obtained using Mathematica.

Using an analogous procedure to the above, we can define a polynomial $Z_L(p)$ for $h=0$ by replacing the α_k above by

$$\beta_k = \binom{N}{k}\overline{\beta}_k\,, \tag{4.7}$$

where $\overline{\beta}_k$ is the average value of $\det A'(k)/\det A'(0)$, $A'(k)$ is A' for G with k bonds of conductivity ϵ, and the normalization factor $1/\det A'(0)$ is to make $Z_L(1)=1$ (otherwise $Z_L(1)$ is huge).

5. Results.

Our principal results are the figures below. Figure 1 (a-e) shows contour plots of $|\sigma_L^*(p)|$ for lattices with sizes ranging from 5×5 to 9×9. In each case, the range of $|\sigma_L^*(p)|$ shown is [0,2], and there are 10 contour levels. One of the main features of these plots is the persistence of a region W in which $|\sigma_L^*(p)|$ is very small. It is known, of course, that $\sigma^*(p)=0$ for $0\le$ p $< p_c$. What is intriguing about the plot is that the vanishing appears to extend in the Im p direction to at least $|\text{Im p}| < 0.1$ in all cases shown, supporting the description of $\sigma^*(p)$ given in the Introduction. Figure 2 shows the fine structure in the 9×9 case, with a range for $|\sigma_9^*(p)|$ equal to [0, 0.1] with 10 contour levels again. Figure 3 shows a three dimensional plot of $|\sigma_L^*(p)|$ for the 9×9 case with vertical range [0,2] again, so that the surface describing $|\sigma_L^*(p)|$ has been chopped off above $|\sigma_L^*(p)|=2$, giving the flat top in the outer fringes seen in the picture.

Here we should make a technical remark about "p_c," i.e., the threshold below which $\sigma_L^*(p)$ "vanishes" for real p. Since we are using $\epsilon=0.001$ and finite L, this threshold is somewhat ill-defined. Furthermore, since we are averaging over realizations of sequential "removals," as long as there is one realization where a conducting path remains as k is increased beyond $N/2$ (or as p is decreased below $p=\frac{1}{2}$), this realization will dominate the average and produce an abnormally low "p_c," as seen in Figure 2. We chose to leave these realizations in to preserve randomness, and because we are only interested in the qualitative behavior of $\sigma^*(p)$, not in determining p_c, which is known to be $\frac{1}{2}$.

One feature of the graph of $|\sigma_L^*(p)|$ which can be seen in Figure 1 to a certain extent, and to a greater extent in plots having a much larger range, is that at the outer fringes of the plots, $|\sigma_L^*(p)|$ is growing very rapidly – the contours are very close together. At this point it is not clear if $\sigma^*(p)$ really has some sort of pole structure on this outer rectangular ring, as indicated in the 8×8 and 9×9 case, or if this is a manifestation of the series expansion (2.1) that we have used. It would be very interesting to plot $\sigma^*(p)$ via (3.2) with $s=1$ to see if this divergent structure persists. However, the determination of the $\mu_n(p)$ is somewhat more involved than finding the α_k in (2.1).

In addition to the figures shown here, we have analyzed the zeros of $\sigma_L^*(p)$ by plotting the zero contours of $\text{Re}[\sigma_L^*(p)]$ and $\text{Im}[\sigma_L^*(p)]$, and finding where they intersect. The zeros seem to congregate on the fringes in the divergent structure, and somewhat in the region W. We have found, however, no evidence of the zeros lying on any particular curves through p_c, as would be the case in a Lee-Yang type transition.

Finally, in Figure 4 we show a contour plot of the fine structure (range = [0,0.1]) of $|\widetilde{Z}_L(p)|$ for $L = 9$, where $\widetilde{Z}_L(p)$ is defined by (2.1) with the α_k replaced by $(\beta_k)^{1/15}$. (We have taken the 15^{th} root in particular because it forces the transition for $\widetilde{Z}_L(p)$ to occur approximately at $p = \frac{1}{2}$.) The region W for the partition function is similar to that for $\sigma_L^*(p)$, but appears to be somewhat larger.

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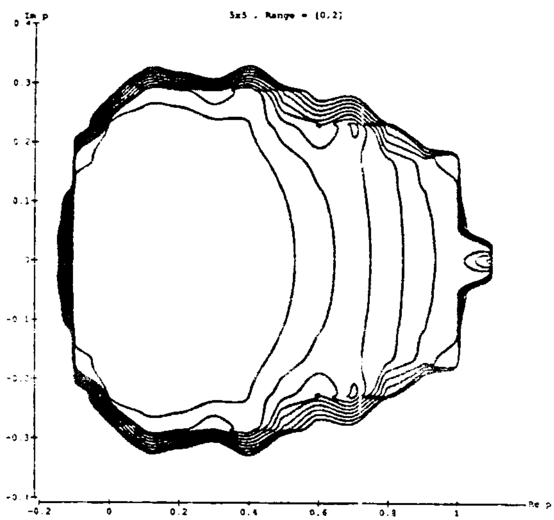

Figure 1a.

Figure 1(a-e). Contour plots of $|\sigma_L^*(p)|$ for $L = 5, \ldots, 9$, with 10 contour levels over a range of [0,2] in each case.

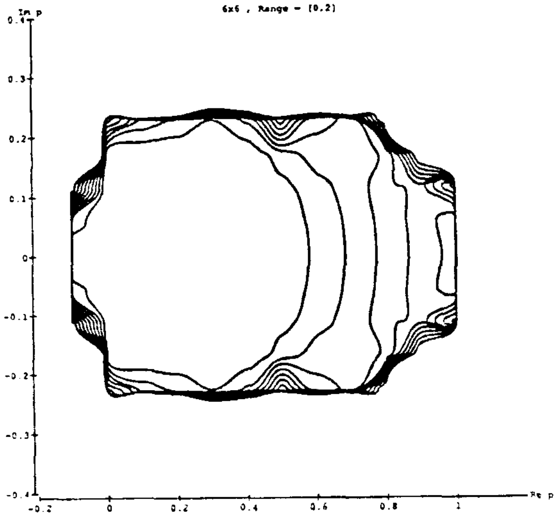

Figure 1b.

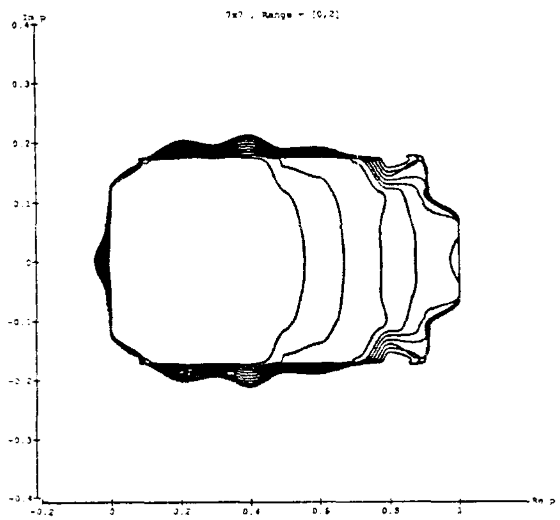

Figure 1c.

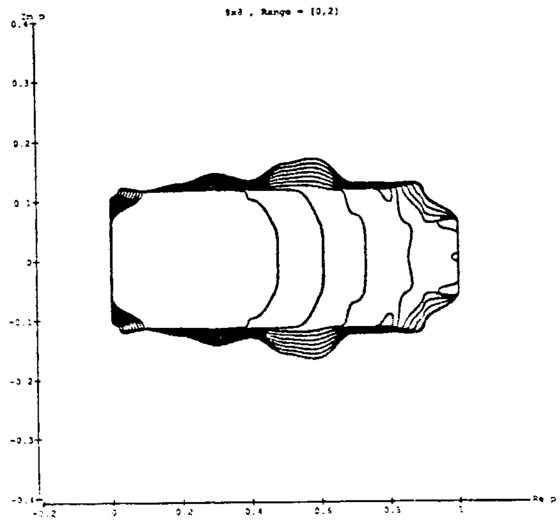

Figure 1d.

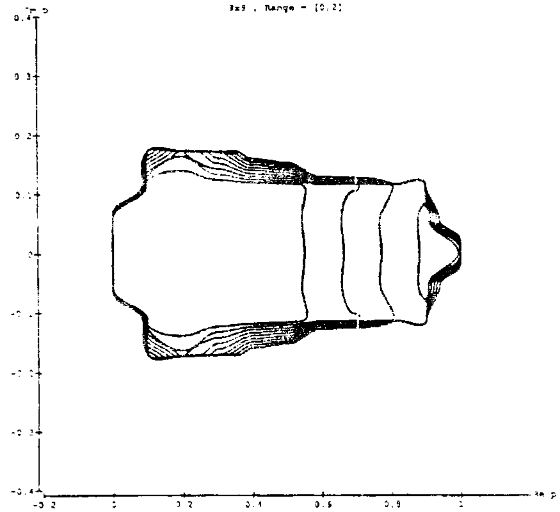

Figure 1e.

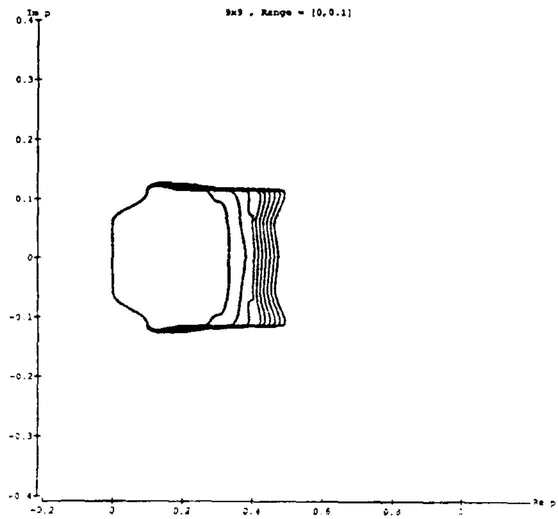

Figure 2. Contour plot of $|\sigma_L^*(p)|$ for $L = 9$ with 10 contour levels over a range of [0,0.1].

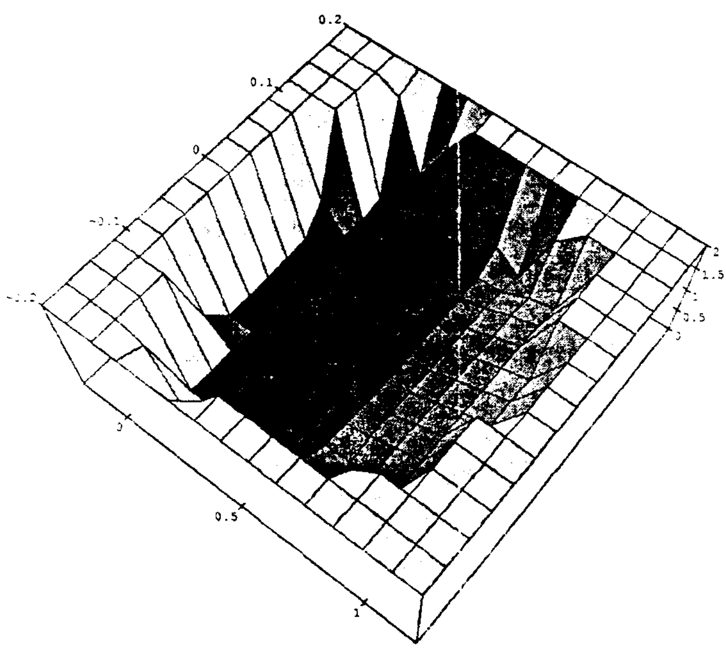

Figure 3. Three dimensional plot of $|\sigma_L^*(p)|$ for $L = 9$ with vertical range [0,2], corresponding to Figure 1e.

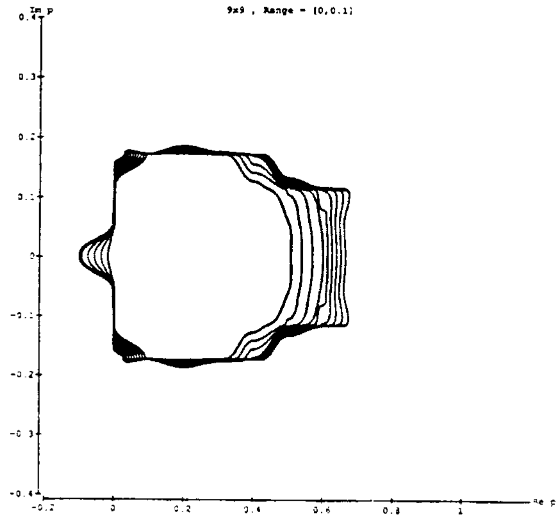

Figure 4. Contour plot of $|\widetilde{Z}_L(p)|$ for $L = 9$ with 10 contour levels over a range of $[0,0.1]$.

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