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Fractal properties of equipotentials close to a rough conducting surface

D O Cajueiro†, V A de A Sampaio†, C M C de Castilho†‡§ and R F S Andrade†

† Instituto de Física, Universidade Federal da Bahia, Campus da Federação, 40210-340 Salvador, Brazil

‡ Department of Chemistry, University of Cambridge, Cambridge CB2 1EW, UK

E-mail: caio@ufba.br (C M C de Castilho)

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Abstract. The Koch curve is used in the problem of evaluating and characterizing the electric equipotential lines in the infinite semi-space limited by a rough conducting one-dimensional surface. The solution of Laplace's equation subject to a constant potential difference between the curve and a straight line placed at infinity is performed with the help of Liebmann's method. The fractal dimension, D_f, of the equipotentials is numerically evaluated with a box-counting method. It is found that D_f decays exponentially with distance, from the value $D_f = 1.273$ at the Koch curve to the $D_f = 1.0$ when the equipotentials become flat smooth lines. The method does not depend on the specific choice of the Koch curve to model the rough substrate.

1. Introduction

Understanding the behaviour of the electric potential and field close to surfaces is necessary for the interpretation of several phenomena present in a plethora of experimental techniques which have been used for the last two or three decades (Woodruff and Delchar 1994, Rivière 1990). Field ionization in the field ion microscope and field desorption or evaporation of atoms and ions in the field desorption microscope and atom probe (Miller *et al* 1996) are just two clear examples. As a result of that, potential and field determination at points close to a structured surface on an atomic scale for even simplified models gives important clues for the interpretation of such phenomena. In such conditions electric field intensity variation close to the surface on an atomic scale (a few ångströms) along a direction 'parallel' to the surface can be significant and interfere in the imaging process. On the other hand, a simultaneous smoothing in its local variation is observed as the distance perpendicular to the sample is increased. So, the important field variation used for creating contrast in the various imaging processes occurs in a somewhat narrow zone close to the surface. The determination of the extension of the zone with a rapid variation of the field becomes then an important issue for this and other similar problems.

In this paper we address the problem of evaluating and characterizing equipotential lines close to a rough one-dimensional conductor surface, whose protrusions and cavities are modelled by the well known Koch fractal. The use of fractal geometry in problems of

§ Corresponding author.

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condensed matter physics with scale invariance, as in the case of a rough surface, is now quite common.

Far away from the Koch curve, a straight line, representing the profile of a metallic plane, is the opposite limit of the region where the electric potential and field intensities are to be calculated. They are then numerically determined in this region, bounded by these two 'metallic lines' which in turn are assumed to be at constant but different potentials. The equipotential lines are calculated and characterized by their fractal dimension, which is evaluated by the well known box-counting method. The ultimate purpose is to describe the dependence of their fractal dimension with respect to the potential strength and to the mean distance to the Koch curve profile. So we can measure the size of the stripe near to the surface where the field and potential have a strong dependence with position, before reaching the region of constant field far away from the surface. The solution of Laplace's equation close to fractal objects is important also for other problems like DLA, where it describes the growth probability of the substrate. Hence the techniques explored here can also be applied to other situations. The choice of the Koch curve to mimic the surface profile has no particular influence on our results. We will use it for it is a well known object and its fractal dimension is known exactly. We could have chosen other geometric fractal or any profile obtained by numerical experiments of surface growth based on simple SOS (solid-on-solid).

The rest of this paper is organized as follows: in section 2 we describe the method used for the solution of Laplace's equation. A brief comment on the concepts of fractal geometry that are used for the determination of the fractal dimension of the equipotentials is provided in section 3, but we omit the details of the box counting algorithm. In section 4 we present our results, closing the paper with some remarks in section 5.

2. Solution of the electric potential

Electric field and equipotentials are important quantities in surface imaging techniques. Frequently the local variation of such quantities on an atomic scale must be determined in order to properly interpret experimental data. The effect of a single protrusion in a smooth surface has been modelled in such a way that analytical and or numerical methods can be used (Homeier and Kingham 1983, Miller *et al* 1996). However, when the surface presents irregularities the problem becomes more difficult, and it is necessary to resort exclusively to a numerical approach for solving Laplace's equation:

$$\nabla^2 V = 0. \tag{1}$$

This equation presents an analytical solution just in cases of highly symmetric boundary conditions (Morse and Feshbach 1953). For solving it numerically in a region limited by two surfaces with constant but different potentials we have used the so-called Liebmann method (Gerald and Wheatley 1984). Such a method substitutes the partial derivatives for a ratio of differences and the following steps are necessary for its implementation:

(1) the domain (the region confined between the two lines/surfaces with constant but different potentials) is divided into a grid;
(2) initial values for the potential are almost arbitrarily attributed at each one of the grid's internal points, obeying the condition that these values are set between the values previously taken for the potential at the boundaries, in this case the Koch curve and a far away straight line 'parallel' to the first stage of the fractal curve;
(3) the potential at the lateral vertical lines, which also bounds the domain, are also fixed, but in this case in a linear variation between the values of the potentials at the Koch curve and at the far away straight line;

(4) to each point of the domain we associate a property, called state, designed as 'FIX' for points where the potential is kept unaltered, i.e. at the boundaries of the grid, or 'FREE' for points where the potential is recalculated by an iterative procedure;
(5) the potential is then calculated at each node. This is done by considering Laplace's equation in the form:

$$\nabla^2 V = \partial^2 V/\partial x^2 + \partial^2 V/\partial y^2 \tag{2}$$

which leads to:

$$\nabla^2 V[I, J] = \{V[I+1, J] + V[I-1, J] - 2V[I, J]\}/\Delta x^2 + \{V[I, J+1] + V[I, J-1] - 2V[I, J]\}/\Delta y^2. \tag{3}$$

In the above equation, taking $\Delta x = \Delta y = h$ we obtain:

$$\nabla^2 V[I, J] = \{V[I+1, J] + V[I-1, J] + V[I, J+1] + V[I, J-1] - 4V[I, J]\}/h^2 \tag{4}$$

where a typical situation for points I, $I+1$, J and $J+1$ can be seen in figure 1.

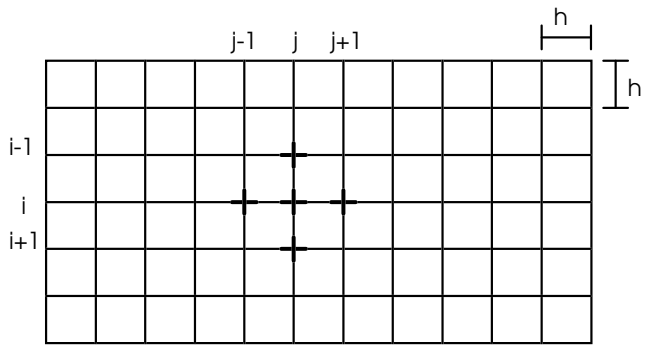


Figure 1. Basic discretized square grid used for the solution of the Laplace equation according to Liebmann's method. In an isometric version, the horizontal and vertical distances are different from each other.

The boundary conditions are then imposed by keeping constant the potential at the points of the grid's contour (Koch curve, where $V = 0$; straight horizontal line far away from the curve, where $V = V_0 > 0$; and the two lateral vertical lines, where V varies linearly with height from $V = 0$ to $V = V_0$), and the process is done iteratively until the maximum difference in successive iterations, at any point, becomes smaller than a previous adopted value, chosen as a convergence criterion. In the present work, the adopted convergence criterion was the maximum percentage change in the local potential between successive iterations, for the set of points where the potential is allowed to vary. Note that in the current problem we could also apply lateral periodic boundary conditions, which avoids the necessity of assigning values for V at the points of the lateral vertical boundaries, but the results are essentially the same.

3. Fractals and fractal dimension

In the last two decades fractal concepts have become well known tools in the analysis of self-similar objects that are invariant under contractions or dilations (Feder 1988). The exact geometrical fractals are ideal objects that satisfy true scale invariance at all sizes. Actual

objects display, in most cases, scale invariance in a restricted region of the length scale and in a statistical sense only. Nevertheless, we can evaluate with high confidence their various different dimensions, which are the most important measures within fractal geometry.

One of the most used numerical methods for computing D is based on covering the object with a grid of boxes that have linear size ε and on counting the number of boxes $N(\varepsilon)$ that contain at least a point of the fractal. This is done for several values of the scale $N(\varepsilon)$. The fractal dimension is determined by the slope of a log–log plot based on the following expression:

$$D_f = -\log[N(\varepsilon)]/\log(\varepsilon). \tag{5}$$

Several highly efficient algorithms are available for the evaluation of the fractal (D_f) and multi-fractal dimensions $D(q)$. Usually they require, as input data, the coordinates of the points of the sets. These coordinates can be obtained after a process of numerical evaluation, as in the present case, or from the digitization of a picture set. We have used the algorithm proposed by Block *et al* (1990), which has shown to be quite reliable in the analysis of fractal sets.

4. Calculations and results

Our calculations were performed in a Cray Y-MP computer with 330 mflops and a 6 ns clock, with a SUN 4/470 as the front-end unit. The successive stages (from first to fourth) of the Koch curve and other boundary lines of the domain are shown in figure 2. We have used both a square grid, with 54 200 points (271 $\times$ 200), and an isometric (rectangular) one, for which we have used 31 436 (271 $\times$ 116) and also 124 971 points (541 $\times$ 231). This is then the grid of points for which equation (4) is iteratively solved. The necessary number of iterations for the assumed convergence (a percental variation) to occur and the used CPU time for each stage for which the potential was calculated are shown in table 1.

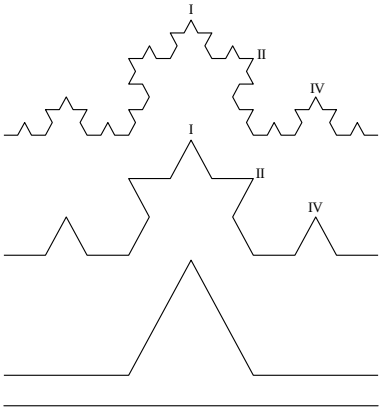


Figure 2. The first four stages of construction of the Koch curve. The true fractal is obtained after an infinite number of iterations. The use of a series of figures based on a finite number of iterations for the analysis of physical phenomena indicates what features are expected for higher order iterations.

It was possible to observe the necessity of using an array of points for the grid with a unit cell that properly matches the geometry of the Koch curve. The use of a grid with a symmetry compatible with that of the boundary (isometric instead of a square one in our case) is essential

Table 1. Performance for a maximum error of 10^{-13}% between successive iterations.

Number of iterations	Computational time (CPU) (s)	Points	Stage	Grid
34 426	1042	31 436 (271×116)	2nd	Isometric (rectangular)
30 678	908	31 436 (271×116)	3rd	Isometric (rectangular)
29 825	874	31 436 (271×116)	4th	Isometric (rectangular)
81 571	4171	54 200 (271×200)	3rd	Square
112 845	13 207	12 4971 (541×231)	4th[a]	Isometric (rectangular)

[a] Grid with an area four times smaller than others.

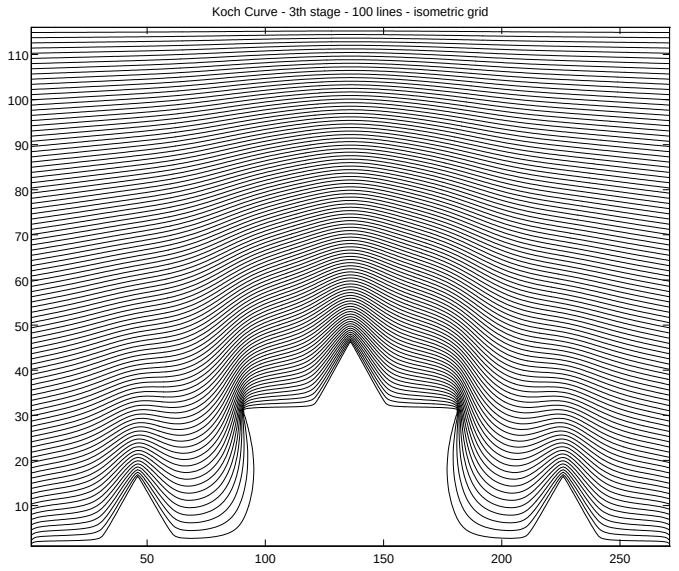
Table 2. Intensity of the electric field components (arbitrary units) at points I, II, IV (see figure 2 for the Koch curve) for an isometric grid for several directions.

	Point I				Point II			Point IV		
Direction	Step 2	Step 3	Step 4	Step 4[a]	Step 3	Step 4	Step 4[a]	Step 3	Step 4	Step 4[a]
Vertical	4.032	3.796	3.424	4.070	3.272	3.034	3.908	2.593	2.337	2.776
Horizontal right	4.336	4.076	3.643	4.362	—	—	—	2.758	2.466	2.962
Horizontal left	4.336	4.076	3.643	4.362	9.165	8.219	11.45	2.806	2.505	2.989
60 with vertical right	4.534	4.265	3.827	4.568	2.083	1.942	2.426	2.891	2.595	3.104
60 with vertical left	4.534	4.265	3.827	4.568	5.664	5.180	6.955	2.933	2.629	3.128

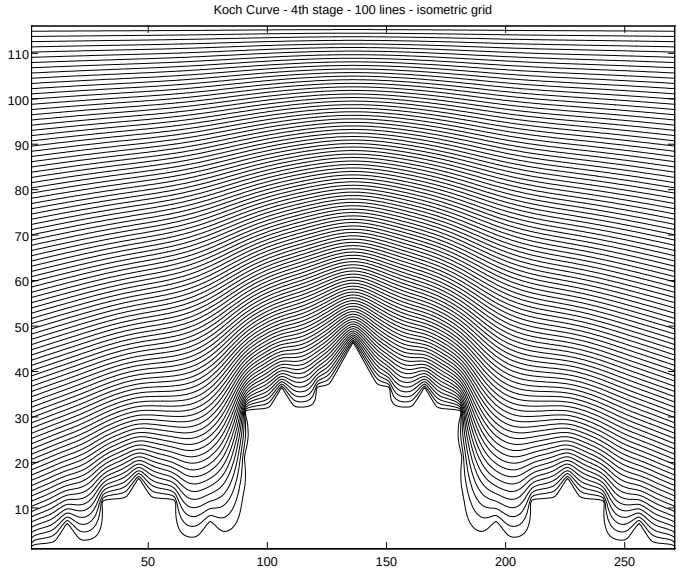
[a]Grid with an area four times smaller than others.

as a way to assure a really constant potential along the curve and also compatibility with the lateral boundary. This also reduces the CPU time and the number of necessary iterations for a chosen convergence parameter to be achieved. At the apex of the Koch curve (point I) the direction of strongest electric field (considering the potential increment between the value at the Koch curve and the one at the closest point of the grid) is not the vertical, as shown in table 2. However, this perhaps is not realistic and just is a result from the discontinuity of the points. A similar effect is observed in the neighbourhood of other corner sites of the boundary. For successive steps in the construction of the curve it was observed that the electric field intensity at a fixed point, provided we use the same grid, is reduced. However, the ratio between field intensities at equivalent points in successive steps is kept constant. For different steps of the curve and for an adequate grid (isometric in our case) the CPU time remains essentially the same. From the third step, it is possible to observe regions (within the cavities increasingly formed as we go through the successive steps of construction) of almost constant potential, i.e. points with a very small field intensity, as can be seen in Figures 3(a) and (b), where the general forms of the equipotentials for the third and fourth stages are represented.

The fractal dimension of the equipotential curves was determined by the already mentioned efficient box-counting algorithm (Block *et al* 1990), where the number of operations required to analyse a set of N points increases only with $N \log_2(N)$. Among several tests performed with the program, we evaluated D_f for the Koch curve. The obtained value, $D_f = 1.258$, agrees



(a)



(b)

Figure 3. Equipotentials obtained for the 3rd (a) and 4th (b) stage of construction of the Koch curve. Note the direction of the most intense field is not along the vertical direction.

with the exact one (log4/log3), with a precision of 0.25%. As expected, the results show that, when the value of the equipotentials grows, the value of its fractal dimension falls, indicating that the equipotentials become smoother, with a shape of a regular Euclidean contour.

Besides this, we have also measured the average vertical distance L from the equipotential lines to the closest point of the surface substrate (Koch curve) with the same horizontal coordinate. We express this distance in units of the maximum height of the Koch curve.

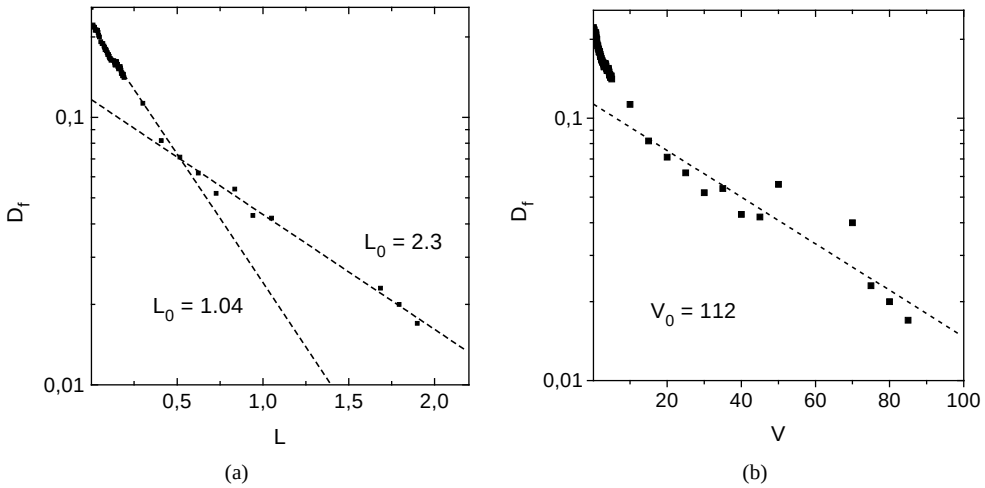


Figure 4. Dependence of the fractal dimension D_f of equipotentials with respect to the value of the distance L (a) and potential V (b).

We have found that, for $0 < L < 0.25$, L increases with V as $L \sim V^{0.82}$. Later it goes through a crossover zone until it reaches a linear dependence, $L \sim 0.021V$. So it is also possible to analyse the dependence of D_f with respect to the mean distance of the equipotential to the boundary. As shown in figure 4, the dependence of D_f on L follows an exponential decay:

$$D_f(L) - 1 = A \exp(-L/L_0) \tag{6}$$

with $L_0 = 1.04$ at least for $L < 0.5$. For $L > 0.5$, D_f decays slower, possibly exponentially, with $L_0 = 2.3$. As the dependence between L and V is roughly linear for $V > 10$, $D_f(V)$ decays also in an exponential way with $V_0 = 112$.

The above figures characterize the size of the stripe close to the surface where the equipotentials and electric fields vary in an irregular way. It is seen that for $L > 1.0$ the value of D_f is already 1.04, which corresponds to a less than 20% departure of the fractal dimension of the Koch curve with respect to that of a smooth line.

5. Conclusions

In this work we have investigated the problem of characterizing the electric potential and field in the region bounded by a Koch curve and a straight line placed far away, with the assumption that the curve and line are conducting media submitted to a potential difference. The problem models the actual physical situation where a rough surface of metal is submitted to an external field, as is the situation of several experimental situations for surface analysis. The problem was addressed in two steps, both of which require the use of numerical methods. In the first one, the solution of Laplace's equation was obtained with Liebmann's method. The solution gives the exact picture of the dependence of the potential with respect to the space. In the second step we could obtain a quantitative dependence of the fractal dimension of the equipotentials with respect to potential value and mean distance to the Koch curve. We have shown that D_f decays exponentially to the limit value $D = 1$ with respect to both potential strength and mean distance. This gives a definite value for the width of the stripe near to the Koch curve where the field varies in a rapid, almost erratic, way.

As already pointed out in the introduction, the choice for the Koch profile plays no definitive role. With it we can investigate other configurations, e.g., placing the Koch curve upside down, mimicking the problem of the field within the cavity of a porous medium. The use of randomly generated profiles obtained according to a SOS (solid-on-solid) scheme can also be used. In such a case, however, the profile is no longer an exact fractal, but it displays self-affinity in an statistical sense. For such situations, the box-counting process used here for the evaluation of the fractal dimensions should be replaced by an equivalent algorithm for the evaluation of the rugosity exponent (Feder 1988, Moreira *et al* 1994). Work in these two directions is in progress.

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