



Modified van der Pauw method based on formulas solvable by the Banach fixed point method

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ABSTRACT

We propose a modification of the standard van der Pauw method for determining the resistivity and Hall coefficient of flat thin samples of arbitrary shape. Considering a different choice of resistance measurements we derive a formula which can be numerically solved (with respect to sheet resistance) by the Banach fixed point method for any values of experimental data. The convergence is especially fast in the case of near-symmetric van der Pauw configurations (e.g., clover shaped samples).

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1. Introduction

The van der Pauw four probe method is a standard technique for measuring the resistivity of flat thin samples of arbitrary shape [1,2]. The sample has to be homogeneous, isotropic, of uniform thickness and simply connected (i.e., without isolated holes). Four contacts placed on the sample are required. They have to be geometric points located on the boundary of the sample (or, in practice, errors caused by their finite size should be sufficiently small).

The van der Pauw geometry is very popular in electric measurements and found a lot of applications in physics, compare, e.g., [3–8]. The method consists in performing direct measurement of resistances $R_{12,34}$ and $R_{23,14}$ (for more details see the next section), and then using the formula

$$\exp\left(-\frac{\pi d R_{12,34}}{\rho}\right) + \exp\left(-\frac{\pi d R_{23,41}}{\rho}\right) = 1 \quad (1)$$

for computing the resistivity ρ and sheet resistance $R_s = \rho/d$ of the sample of thickness d . Then, the Hall coefficient is computed as

$$\mu_H = \frac{\Delta R_{24,13}}{B R_s}, \quad (2)$$

where $\Delta R_{24,13}$ is the change of $R_{24,13}$ due to the magnetic field B . Eq. (1) is believed to be unsolvable by the fixed point method. Usually, instead of numerical procedures, a graph of the so called geometric factor is used to determine a solution of Eq. (1). Some authors recommend to

use tables of numerical values of this function [9]. An inherent inaccuracy of these methods seems to be commonly recognized.

Many attempts have been made to develop and improve the van der Pauw approach, see [10–18]. However, the formula (1) has always been treated as a starting point. In this paper we will show that another formula, namely:

$$\exp\frac{\pi d R_{\max}}{\rho} - \exp\left(\frac{\pi d |R_{24,13}|}{\rho}\right) = 1, \quad (3)$$

(where $R_{\max} = \max\{R_{12,34}, R_{23,41}\}$),

can be used instead of Eq. (1). We will show that preconditions for the Banach fixed point theorem are rigorously satisfied for any set of experimental results, usually with an excellent rate of convergence.

Our approach is especially convenient in Hall effect measurements with symmetric (or near-symmetric) van der Pauw configuration (e.g., in the shape of a clover leaf). In the symmetric case $R_{24,13} = 0$ and, therefore, formula (3) yields the well known explicit expression: $\rho = \pi d R_{\max} / \ln 2$. In near-symmetric cases $R_{24,13}$ is much smaller than R_{\max} and we need just few iterations to get very accurate numerical results.

2. A brief review of the van der Pauw method

The main idea of the van der Pauw approach is simple and beautiful. First, one considers a sample in the form of the complex upper half plane (with contacts placed on the real axis). All computations can be explicitly done in this case. Then, one applies a deep mathematical theory (the Riemann mapping theorem) showing that any

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other (simply connected) sample is conformally equivalent to the upper half plane [19]. What is more, this conformal transformation preserves all equipotential lines, current lines and boundary conditions [1]. Therefore any formula which does not contain explicit information about positions of contacts is invariant with respect to such transformations, and results obtained in the case of the half plane are exactly valid for samples of arbitrary shape (provided that they have no isolated holes).

Therefore, we consider the upper half plane, parameterized by complex coordinate z ($\text{Im}z \geq 0$). Four contacts are represented by x_1, x_2, x_3, x_4 lying on the real axis. In order to perform a measurement we inject electric current J_{jk} at contact x_j , take it out at x_k ($k \neq j$), and measure the voltage between remaining two points. Elementary considerations (based on the superposition principle) show that electric potential at z is given by

$$\Phi(z) = \frac{J_{jk}\rho}{\pi d} \ln \left| \frac{z - x_k}{z - x_j} \right| \quad (4)$$

(note that $|z_1 - z_2|$ is a distance between complex numbers z_1 and z_2). There are $4! = 24$ different ways to perform measurements described above. In any case we compute a resistance

$$R_{jk,mn} = \frac{\Phi(x_n) - \Phi(x_m)}{J_{jk}} = \frac{\rho}{\pi d} \ln \left| \frac{(x_n - x_k)(x_m - x_j)}{(x_n - x_j)(x_m - x_k)} \right|, \quad (5)$$

where j, k, m, n are pairwise different (a permutation of 1, 2, 3, 4) and it is convenient to denote $R_s = \rho/d$ (sheet resistance). Thus we have 24 relations between x_1, x_2, x_3, x_4 and R_s , treated as unknowns. $R_{jk,mn}$ are calculated directly from experimental data. Eliminating x_1, x_2, x_3, x_4 van der Pauw obtained Eq. (1) valid for samples of arbitrary shape, compare [1,2]. We stress that the exact placement of contacts on the circumference of the sample is not important with exception of their ordering.

In the next section we study consequences of Eq. (5) in more detail. In particular, we derive Eq. (3).

3. Modification of the van der Pauw method

In the formula (5) one can recognize the cross ratio, a well known and very important notion in projective geometry. The cross ratio of four (ordered) points x_j, x_k, x_m, x_n is defined as

$$(x_j, x_k; x_m, x_n) := \frac{(x_m - x_j)(x_n - x_k)}{(x_m - x_k)(x_n - x_j)}. \quad (6)$$

The same formula applied for a 4-tuple of complex numbers is used in conformal (Möbius) geometry [19,20]. There exists a natural generalization of the cross ratio on points in Euclidean spaces of any dimension [21].

Taking into account Eq. (6) we rewrite Eq. (5) as

$$\pi R_{jk,mn} = R_s \ln |(x_j, x_k; x_m, x_n)|. \quad (7)$$

Cross ratios corresponding to various permutations of four points x_1, x_2, x_3, x_4 are related by a set of identities which can be shortly written as:

$$(x_j, x_k; x_m, x_n) = (x_m, x_n; x_j, x_k) = (x_j, x_k; x_n, x_m)^{-1}, \quad (8)$$

$$(x_j, x_k; x_m, x_n) + (x_j, x_m; x_k, x_n) = 1, \quad (9)$$

(they can be verified by straightforward elementary calculation). In particular, on use of Eqs. (8) and (9) we easily derive the following equations

$$(x_1, x_2; x_3, x_4)^{-1} + (x_2, x_3; x_4, x_1)^{-1} = 1, \quad (10)$$

$$(x_1, x_2; x_3, x_4) + (x_2, x_4; x_1, x_3) = 1, \quad (11)$$

$$(x_2, x_3; x_4, x_1) + (x_2, x_4; x_1, x_3)^{-1} = 1. \quad (12)$$

Taking into account Eq. (7), and assuming (without loss of the generality)

$$x_1 < x_2 < x_3 < x_4, \quad (13)$$

we obtain corresponding identities for resistances $R_{jk,mn}$ (in Appendix A we present another approach, where inequalities (13) are not assumed). Eqs. (8) yield the so called reciprocal and reversed polarity identities, for instance:

$$R_{12,34} = R_{34,12} = R_{21,43} = R_{43,21}. \quad (14)$$

They are useful for eliminating some side effects (one takes an average of the above four measurements instead of $R_{12,34}$, etc.). In our approach improvements of this kind can be done in exactly the same way as in the standard van der Pauw method. Note that inequalities (13) mean that contacts x_1, x_2, x_3, x_4 are placed in exactly this order (counterclockwise) on the circumference of the sample.

Cross ratios are not necessarily positive. Using Eqs. (6) and (13) we can determine signs of cross ratios. Moreover, Eq. (10) implies upper bounds on both (positive) components. Thus:

$$\begin{aligned} (x_1, x_2; x_3, x_4) &> 1, \\ (x_2, x_3; x_4, x_1) &> 1, \\ (x_2, x_4; x_1, x_3) &< 0. \end{aligned} \quad (15)$$

Eq. (10) yields van der Pauw's formula (1). Surprisingly enough, Eqs. (11) and (12) lead to the following, physically meaningful, formulas:

$$\exp(\pi R_{12,34}/R_s) - \exp(\pi R_{24,13}/R_s) = 1. \quad (16)$$

$$\exp(\pi R_{23,41}/R_s) - \exp(-\pi R_{24,13}/R_s) = 1. \quad (17)$$

For further analysis we choose the first equation if $R_{24,13} > 0$ or the second equation if $R_{24,13} < 0$. In the first case we have $R_{12,34} > R_{23,41} > 0$, while in the second case $R_{23,41} > R_{12,34} > 0$. Both cases can be shortly represented as Eq. (3) where R_{\max} denotes greater of two values: $R_{12,34}$ or $R_{23,41}$.

4. Fast converging numerical iterations

Eq. (3) can be rewritten as:

$$x = \ln(1 + e^{kx}), \quad k = \frac{|R_{24,13}|}{R_{\max}}, \quad (18)$$

where $x = \pi R_{\max}/R_s$. The discussion at the end of the previous section shows that $0 \leq k < 1$.

Eq. (18) has a form $x = F(x)$, characteristic for the Banach fixed point method. In order to obtain a solution (the fixed point of the map F) one has to iterate: $x_{n+1} = F(x_n)$. We are going to show that function $F(x) = \ln(1 + e^{kx})$ satisfies preconditions for the Banach fixed point theorem (for any k). Indeed, F maps segment $L_k = [\ln 2, \frac{\ln 2}{1-k}]$ into itself because:

$$\begin{aligned} x \geq \ln 2 &\Rightarrow F(x) \geq \ln(1 + 2^k) \geq \ln 2, \\ x \leq \frac{\ln 2}{1-k} &\Rightarrow F(x) \leq \frac{k \ln 2}{1-k} + \ln 2 = \frac{\ln 2}{1-k}, \end{aligned} \quad (19)$$

where we took into account $F(x) = kx + \ln(1 + e^{-kx})$. Then,

$$|F'(x)| = \frac{k}{1 + e^{-kx}} \leq k \quad (20)$$

for any $x \in L_k$. Therefore, by virtue of the Lagrange mean value theorem

$$\frac{|F(x_1) - F(x_2)|}{|x_1 - x_2|} = |F'(c)| \leq k < 1 \quad (21)$$

(for any $x_1, x_2 \in L_k$) which means that F is a contraction of the segment L_k .

In order to estimate the number of iterations N needed to obtain a prescribed accuracy δ we require that the length of the segment after applying N contractions is smaller than δ :

$$\frac{k^{N+1} \ln 2}{1-k} \leq \delta \Rightarrow N \approx \frac{\ln\left(\frac{(1-k)\delta}{k \ln 2}\right)}{\ln k}. \quad (22)$$

The actual number of iterations is, of course, much smaller. Table 1 shows the number of iterations needed to obtain the accuracy $\delta = 10^{-5}$. For k approaching 1 the number of iterations increases (tending to infinity). In this region ($k \approx 1$) it is better to use another iterating scheme, see below. Note that as an initial point we took $x_0 = \ln 2$ (this is almost obligatory for small k , when the length of segment L_k is very small and only $x_0 = \ln 2$ belongs to any L_k). Table 1 contains also corresponding values of the relative sheet resistance \hat{R}_s defined by

$$\hat{R}_s = \frac{R_s}{R_{\max}} = \frac{\pi}{x}, \quad (23)$$

where x is the solution of Eq. (18).

Multiplying equation $e^x = 1 + e^{kx}$ (equivalent to Eq. (18)) by e^{-x} we get: $e^{-x} = 1 - e^{-kx}$. Hence we have another form of Eq. (18):

$$x = -\ln(1 - e^{-k'x}), \quad k' = 1 - k. \quad (24)$$

One can rigorously show that preconditions for the Banach fixed point method are satisfied (at least for sufficiently small k' , namely $k' < 0.125$) provided that as a starting point we take $x_0 = -\ln k'$ (in practice, the Banach method seems to work very well for larger range of k' , at least up to $k' \approx 0.25$). We omit technical details. Instead, we present Table 2 showing that for small k' (i.e., $k \approx 1$) Eq. (24) is excellently solvable by the fixed point method.

5. Summary

In this paper we proposed an alternative approach to the standard van der Pauw method. Measurements are essentially the same as in the standard method and produce three resistances: $R_{12,34}$, $R_{23,41}$, $R_{24,13}$ (reciprocal and reversed resistances can be used for improving the accuracy, compare Eq. (14)). We take $R_{24,13}$ and greater of remaining two resistances, denoting it by R_{\max} . Then we compute two coefficients: $k = |R_{24,13}|/R_{\max}$ and $k' = 1 - k$. In order to find the

Table 1

Number of iterations N necessary to obtain solution x of Eq. (18) ($x_0 = \ln 2$, $\delta = 10^{-5}$) and $\hat{R}_s = R_s/R_{\max}$ as a function of $k = |R_{24,13}|/R_{\max}$.

k	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
N	1	4	5	6	7	9	12	15	24	42
\hat{R}_s	4.532	4.302	4.062	3.811	3.546	3.264	2.960	2.623	2.234	1.743

sheet resistance we solve either (18) (for $0 \leq k < 0.9$) or (24) (for $0.8 < k < 1$) and calculate $R_s = \pi R_{\max}/x$. In the indicated ranges of k both equations are solvable by the Banach fixed point method with excellent rates of convergence.

Analysing theoretical consequences of the van der Pauw approach we derived formulas which are solvable by fast convergent numerical algorithm. We used exactly the same assumptions and data as required by the original van der Pauw method. Therefore, any results obtained by our method should be identical with those produced by the standard approach (provided that all van der Pauw assumptions are satisfied with sufficient accuracy).

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Appendix A

It is convenient to rewrite cross ratio identities in terms of resistances. Using Eq. (7) we transform Eqs. (8) and (9) into:

$$R_{jk,mn} = R_{mn,jk} = -R_{jk,nm}, \quad (25)$$

$$\varepsilon_{jk,mn} \exp\left(\frac{\pi}{R_s} R_{jk,mn}\right) + \varepsilon_{jm,kn} \exp\left(\frac{\pi}{R_s} R_{jm,kn}\right) = 1, \quad (26)$$

where $\varepsilon_{jk,mn} = \pm 1$ and $\varepsilon_{jm,kn} = \pm 1$. An elementary algebraic analysis shows that $\varepsilon_{jk,mn}$ and $\varepsilon_{jm,kn}$ are uniquely determined by $R_{jk,mn}$ and $R_{jm,kn}$. Indeed, one can distinguish the following cases (we assume $R_{jk,mn} \geq R_{jm,kn}$):

$$R_{jk,mn} < 0 \Rightarrow \varepsilon_{jk,mn} = 1, \varepsilon_{jm,kn} = 1, \quad (27)$$

$$R_{jk,mn} > 0 \Rightarrow \varepsilon_{jk,mn} = 1, \varepsilon_{jm,kn} = -1. \quad (28)$$

$$R_{jk,mn} = 0 \Rightarrow \varepsilon_{jk,mn} = 1, R_{jm,kn} = -\infty. \quad (29)$$

Here we do not make any assumptions on the ordering of points x_k (e.g., we do not assume inequalities (13)).

Another useful identity can be verified by a straightforward short calculation (or derived from Eqs. (8) and (9)):

$$(x_j, x_k; x_m, x_n)(x_j, x_m; x_n, x_k)(x_m, x_k; x_n, x_j) = -1. \quad (30)$$

In terms of resistances this formula has the form

$$R_{jk,mn} + R_{jm,nk} + R_{mk,nj} = 0, \quad (31)$$

known to van der Pauw, see [1].

We proceed to presenting another modification of the van der Pauw method. Supposing that we measured two resistances: $R_{jk,mn}$ and $R_{jm,kn}$. Without loss of the generality we assume $R_{jk,mn} \geq R_{jm,kn}$ (in the opposite case it is enough to rename contacts, $x_k \leftrightarrow x_m$). We have two distinct cases:

1. $R_{jk,mn} < 0$. Then, by virtue of Eqs. (27), we get the van der Pauw equation

$$\exp\left(-\frac{\pi}{R_s} |R_{jk,mn}|\right) + \exp\left(-\frac{\pi}{R_s} |R_{jm,kn}|\right) = 1, \quad (32)$$

where $|R_{jk,mn}| < |R_{jm,kn}|$. Denoting

$$x = \frac{\pi |R_{jm,kn}|}{R_s}, \quad k = \frac{|R_{jm,kn}| - |R_{jk,mn}|}{|R_{jm,kn}|}, \quad (33)$$

Table 2

Number of iterations N necessary to obtain solution x of Eq. (24) ($x_0 = -\ln k'$, $\delta = 10^{-5}$) and $\bar{R}_s = R_s/R_{max}$ as a function of $k' = 1 - k$.

k'	0.2	0.1	0.01	10^{-3}	10^{-4}	10^{-6}	10^{-8}	10^{-10}	10^{-12}	10^{-15}
N	22	18	10	8	7	5	4	4	4	3
\bar{R}_s	2.234	1.743	0.924	0.598	0.434	0.276	0.200	0.157	0.129	0.101

we obtain $e^x = 1 + e^{kx}$ ($0 < k < 1$) which can be solved by the fixed point method, see Section 4.

2. $R_{jk,mn} > 0$. Then, by virtue of Eq. (28), we get the modified equation

$$\exp \frac{\pi}{R_s} R_{jk,mn} - \exp \frac{\pi}{R_s} R_{jm,kn} = 1, \quad (34)$$

where $R_{jk,mn} > R_{jm,kn}$. Denoting

$$x = \frac{\pi R_{jk,mn}}{R_s}, \quad k = \frac{R_{jm,kn}}{R_{jk,mn}}, \quad (35)$$

we also obtain $e^x = 1 + e^{kx}$ but now $-1 < k < 1$ ($R_{jm,kn}$ can be negative). The case $-1 < k < 0$ can be solved by the fixed point method as well. Actually, for negative k (including $k = -1$) the convergence is much better, because in this case $F'(x)$ is estimated by $\frac{1}{2}|k|$ (instead of $|k|$), compare inequality (20).

We omit the third case ($R_{jk,mn} = 0$), because then $R_{jm,kn} = \infty$, see Eqs. (29). It implies either $x_j = x_k$, or $x_m = x_n$, which contradicts our

assumption that x_k are pairwise different. Note that the symmetric case corresponds to $|R_{jk,mn}| = |R_{jm,nk}|$ (if $R_{jk,mn} < 0$), or to $R_{jm,kn} = 0$ (if $R_{jk,mn} > 0$). Then formulas (32) and (34) have simple exact solutions.

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