Not seeing the roots for the branches: multivalued functions in computer algebra

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Abstract

We discuss the multiple definitions of multivalued functions and their suitability for computer algebra systems. We focus the discussion by taking one specific problem and considering how it is solved using different definitions. Our example problem is the classical one of calculating the roots of a cubic polynomial from the Cardano formulae, which contain fractional powers. We show that some definitions of these functions result in formulae that are correct only in the sense that they give candidates for solutions; these candidates must then be tested. Formulae that are based on single-valued functions, in contrast, are efficient and direct.

1 Introduction

Within the development communities of the various computer algebra systems (CAS), there have been extensive discussions of the best way to define and implement multivalued functions. So far, these discussions have remained largely unpublished, but we believe that their publication is necessary and important. Many of those who have been connected with the development of MAPLE can testify to the uncountable hours absorbed by the (internal) debates surrounding the correction of the "square-root bug", a multivalued-function bug. The wider mathematical community has at present few ways of learning about the conclusions reached during those debates, and yet the experiences of CAS developers should be influencing mathematics and mathematical standards. For example, the Digital Library of Mathematical Functions (http://dlmf.nist.gov) is at present being prepared, and it is desirable that this standard reference be aware of the stance of the CAS community (if it has one) on multivalued functions. The Openmath standard (see http://www.openmath.org) includes principal-value functions [11], but although this standard suits many purposes, it has not reached or influenced the vast body of mathematicians.

There is one area of research in multivalued functions which is slowly developing a body of published literature, and that is the simplification of principal-value functions, see [13, 12, 22, 19, 2, 11, 5, 4, 3]. However, the underlying assumption of the area, namely that the principal value is the best way to implement a multivalued function, is not an assumption that is uniformly accepted outside the CAS community, and perhaps not even within it. In the wider field of mathematics, there are still many reference books and textbooks (and people) that prefer definitions other than principal value.

We think that part of the problem is the manner in which previous discussions have been held. The questions typically debated in the past have been of the form

' does
$$\sqrt{z^2} = z$$
?'

It is natural to ask the question in this form, because this is the sort of equation contained in all the algebra textbooks, and all the reference books. The trouble is that when a group of people start to debate such an equation, every person is correct. One person will give a definition that makes the statement true, and another will give a definition that makes it false, but as long as each system of definitions and implications is consistent, both parties are correct. As a result, the unpublished discussions we have witnessed often fall into predictable patterns. Each person states "When I was an undergraduate in university X, I was always taught that ...". What faith we all have in our particular educations! Further, many discussions assume that human interaction is present. Computer Algebra systems are always striving for greater automation, and that makes a difference.

We wish to introduce a new way of discussing the definitions. Rather than starting with an equation that contains multivalued functions, and then converting it into another equation that contains the same types of functions, we shall start with a problem that does not contain multivalued functions. Further, the required solution does not contain multivalued functions either, and any multivalued functions are introduced only as intermediate expressions during the computations. Then we can ask how the calculation would be implemented in a CAS. Our example problem is the computation of the roots of a cubic equation using the formulae of Cardano [23]. Our equation is $z^3 + 3iz - 2 = 0$. All the quantities appearing are single-valued, and the roots are three unique complex numbers. So our question is how this problem is solved using the different definitions of multivalued functions.

1.1 Things not being discussed

Solving equations is a topic about which everyone has opinions. Thus it is easy for a discussion to become side-tracked, following any number of the most attractive and colourful red herrings. Some readers will want to argue that explicit solutions of polynomial equations are too long and complicated as expressions ever to be useful; they will prefer constructions such as MAPLE'S RootOf. Others will worry about the numerical stability of the formulae; they will prefer to apply Newton's method to the original equation. Still others will baulk when they see the cube root of a complex number appearing in the formulae below; they will maintain that there are no computational circumstances in which one ought ever to try to extract a cube root as part of a formula, especially not a complex one. They would support this by observing that, in the same sense, one should never compute a factorial, since in all cases in which it seems that a factorial is needed, there is some better way to proceed.

All of these objections, and many others, would be interesting paths to follow if the purpose of this article were to solve equations. However, we are not solving equations, we are discussing multivalued functions. The cubic equation is used here as an example which displays the problems of multivalued functions, while being familiar to many readers. The solution formulae are widely quoted — and misquoted — and therefore they are good vehicles for examining multivalued functions.

1.2 Terminology

One of the themes of this paper is clarity in notation and definition, and in order to be clear ourselves, we need to make one distinction in language. We shall be discussing two different sorts of roots in this paper: roots as in square root and cube root, and roots as in places where a polynomial is zero. Since one type of root is going to be expressed in terms of the other type of root, there is a possibility of confusion. Therefore, when we wish to refer generally to square roots, cube roots and similar radicals, we shall call them fractional powers, and reserve the unqualified word root for the place where a polynomial is zero. Notice the difference between a cubic root and a cube root; a cubic root is a place where a cubic polynomial is zero, whereas a cube root is a fractional power.

2 Cardano solution formulae

Before commencing any general discussion, it is best to have the formulae of interest in front of us. If the reduced cubic is written as

$$y^3 + 3py - 2q = 0 (1)$$

then its 3 solutions are given in Abramowitz and Stegun [1] as y_1, y_2, y_3 , where

$$s_1 = \left(q + \sqrt{q^2 + p^3}\right)^{\frac{1}{3}} \,, \tag{2}$$

$$s_2 = \left(q - \sqrt{q^2 + p^3}\right)^{\frac{1}{3}} , (3)$$

$$y_1 = s_1 + s_2 , (4)$$

$$y_2 = -\frac{1}{2}(s_1 + s_2) + i\frac{\sqrt{3}}{2}(s_1 - s_2),$$
 (5)

$$y_3 = -\frac{1}{2}(s_1 + s_2) - i\frac{\sqrt{3}}{2}(s_1 - s_2). \tag{6}$$

To these equations, some authors [14, 15] add the rider

$$s_1 s_2 = -p (7)$$

which clearly shows that they are thinking of the fractional powers as multivalued. In contrast, Maple and Mathematica give, using the same s_1 as above, the solutions Y_1, Y_2, Y_3 , where

$$Y_1 = s_1 - \frac{p}{s_1} \,, \tag{8}$$

$$Y_2 = -\frac{1}{2} \left(1 - i\sqrt{3} \right) s_1 + \frac{1}{2} \left(1 + i\sqrt{3} \right) \frac{p}{s_1} , \qquad (9)$$

$$Y_3 = -\frac{1}{2} \left(1 + i\sqrt{3} \right) s_1 + \frac{1}{2} \left(1 - i\sqrt{3} \right) \frac{p}{s_1} . \tag{10}$$

Some further comments on these formulae are given in an appendix.

2.1 Interpretation of the formulae

Are the above formulae 'right' or 'wrong'? Clearly, it depends upon what the symbols mean. Versions of Maple, up to and including 5.0, used the formulae (2)–(6) to solve cubic equations. When incorrect numerical results appeared, it was natural for Maple developers to brand the formulae as 'wrong'. In reaction, many mathematicians defended the formulae by countering that it was Maple's interpretation that was wrong. The assertion was made that if the radicals, or fractional powers, were interpreted as multivalued functions, then the formulae would be correct.

Therefore, before the correctness of the formulae can be decided, we must be completely clear on what the definitions of the terms are. This brings us back to the purpose of this paper, which is to clarify the possible definitions and to select between them.

3 Definitions and notation

A few quotations are always a good way to start a discussion, so here are ours.

It will be useful, however, for the student to know that ultimately it will be proved that $\sqrt[q]{k}$ has in every case q different values, expressions for which, in the form of complex numbers, can be found

— G. Chrystal, Algebra (1st edition 1889) [9]

In[1] = Sqrt[-2]
Out[1] = i Sqrt[2]
In[2] = N[Out[1]]
Out[2] = 0.+1.41421 i

— Mathematica, Personal communication

'When I use a word,' Humpty Dumpty said in rather a scornful tone, 'it means just what I choose it to mean — neither more nor less.'

'The question is,' said Alice, 'whether you can make words mean different things.'

'The question is,' said Humpty Dumpty, 'which is to be master — that's all.'

— Lewis Carroll, Through the looking glass

It is a mistake to think that square root and cube root do not need to be defined. As an example of how easily confusion can enter, we consider the use of the symbol $\sqrt{}$ in Numerical Recipes §5.6 [21], where there are uncommented, but implied, changes in the meaning of notation. Thus we first read that $ax^2 + bx + c = 0$ has the solution

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \ .$$

The fact that the authors write \pm implies that $\sqrt{}$ has a definite sign. However, after their equation (5.6.6), we read that "the sign of the square root should be chosen so as to make

$$\operatorname{Re}\left(b^*\sqrt{b^2 - 4ac}\right) \ge 0.$$
 (11)

Thus, the symbol $\sqrt{}$ has changed into a multivalued variant. To avoid any doubt, we must start by setting down unambiguous notation that will keep the different definitions separate. We define four separate notations, one for each definition: $\{z^{1/n}\}$, $z^{1/n}$, $\sqrt[n]{z}$, $\operatorname{surd}(z,n)$.

Generally, authors treat notations such as $z^{1/n}$ and $\sqrt[n]{z}$ as synonyms, and choose between them for reasons of convenience or æsthetics. Typically, $\sqrt[n]{z}$ is favoured when z is a short expression, and $z^{1/n}$ when z is lengthy or contains fractions. Notice, for example, just such a mixture in (2)–(3). Here, however, differing notations are used to distinguish different definitions. In the following subsections, it is assumed that the real nth root of a positive real number is already defined.

3.1 Set of values: $\{z^{1/n}\}$

This notation is used for a fractional power treated as a set of values. Thus, given $z \in \mathbb{C}$,

$$\{z^{1/n}\} = \{w \in \mathbb{C} \mid w^n = z\}$$
 (12)

Each value in the set belongs to one branch of the function. $Example: \{(-8)^{1/3}\} = \{-2, 1 + i\sqrt{3}, 1 - i\sqrt{3}\}.$

3.2 One value taken from set: $z^{1/n}$

This notation represents a single number, which, however, retains some indeterminacy, because the branch is not specified.

$$z^{1/n} = |z|^{1/n} \exp\left(\frac{\arg z + 2\pi ik}{n}\right) , \qquad (13)$$

for arg $z \in (-\pi, \pi]$ and for some $k \in \mathbb{Z}$. Note that $|z|^{1/n}$ is a unique real number. $Example: (-8)^{1/3} = 2e^{(2k+1)\pi i/3}$, for k = 0, 1, 2.

3.3 Principal value: $\sqrt[n]{z}$

This notation is used for the single-valued, principal-branch function [10], defined by

$$\sqrt[n]{z} = |z|^{1/n} \exp\left(\frac{\arg z}{n}\right) . \tag{14}$$

Here, $\arg z \in (-\pi, \pi]$, and we allow the default case $\sqrt{z} = \sqrt[3]{z}$. (Questions regarding branch-cut placement and closure are more examples of interesting red herrings [10, 22].) Example: $\sqrt[3]{-8} = 1 + i\sqrt{3}$.

3.4 Real branch: surd(z, n)

MAPLE accommodates users who want the cube root of a negative real to be a negative real by defining a separate function called **surd**. We adopt that notation here. If $x \in \mathbb{R}$, then $\operatorname{surd}(x,3) = \operatorname{sgn}(x)\sqrt[3]{|x|}$, where the cube root is real. More generally, if $z \in \mathbb{C}$ and $n \in \mathbb{Z}$, then $\operatorname{surd}(z,n)$ is the complex nth root whose argument is closest to that of z, with ties being decided by counter-clockwise continuity [17]. $Example: \operatorname{surd}(-8,3) = -2$.

4 Obtaining solutions

We now interpret the Cardano formulae using each of the above definitions in turn. We shall solve the cubic equation $z^3 + 3iz - 2 = 0$ (notice the complex coefficient), and we aim to recover the three solutions z = 1.34201 - 0.86489i, -1.26110 + 1.49918i, -0.08091 - 0.63429i. This accuracy is not necessary, however, and below we specify all numbers by floating-point approximations quoted to 2 decimal places.

4.1 Using sets of values

We rewrite (2) as

$$s_1 = \left\{ \left(q + \left\{ (q^2 + p^3)^{1/2} \right\} \right)^{1/3} \right\} .$$

The computation runs

Therefore s_1 is a set of 6 elements, and this set equals the set s_2 .

4.1.1 Without using rider (7)

Because of the symmetry between s_1 and s_2 , there are 21 elements in the sum, rather than 36. Since we have to identify elements, we have to change from a set to a list.

$$s_1 + s_2 = \begin{bmatrix} -0.64 - 0.43i, -1.29 + 0.09i, -1.13 + 2.32i, -1.26 + 1.50i, 2.57 - 0.18i, \\ -0.51 + 0.39i, -1.45 - 2.14i, -1.42 - 0.73i, -1.39 + 0.68i, -0.67 - 1.84i, \\ 0.08 + 1.60i, 1.34 - 0.87i, 0.59 + 0.25i, 0.56 - 1.16i, 1.28 + 0.87i, \\ 0.72 + 1.07i, 0.11 - 1.55i, -0.06 + 0.77i, -0.08 - 0.63i, 0.70 - 0.34i, 1.93 + 0.34i \end{bmatrix}.$$

The expressions (5) and (6) give the same 21 values. As the title of the paper says, the roots are well hidden by all the branches. To reveal the actual solutions, we now calculate the residuals by substituting each of the 21 values into the original equation. The residuals are

$$\begin{bmatrix} -0.60 - 2.4i, -4.4 - 3.4i, 7.8 - 7.0i, -(4)10^{-9} - (6)10^{-9}i, 15 + 4.1i, -3.1 - 1.3i, 21 - 8.0i, -0.41 - 8.3i, \\ -4.8 - 0.54i, 10 + 1.8i, -7.4 - 3.8i, -(3)10^{-9} + (5)10^{-9}i, -2.6 + 2.0i, -0.62 + 2.1i, -5.4 + 7.5i, \\ -7.3 + 2.6i, 1.8 + 4.0i, -4.2 - 0.62i, (1)10^{-9} + (2)10^{-9}i, -0.88 + 1.6i, 3.5 + 9.6i \end{bmatrix} .$$

In this case, it is easy to identify the 4th, 12th and 19th values as being correct.

4.1.2 Using rider (7)

We compute the list of values of s_1s_2 .

$$\begin{bmatrix} -0.60 - 0.09i, 0.22 + 0.56i, (3)10^{-10} - 1.00i, 0.87 + 0.50i, -0.87 + 0.50i, 0.37 - 0.47i, \\ 0.22 + 0.56i, 0.37 - 0.47i, -0.87 + 0.50i, (3)10^{-10} - 1.00i, 0.87 + 0.50i, -0.56 - 0.09i, \\ (3)10^{-10} - 1.00i, -0.87 + 0.50i, 1.65 - 0.24i, -0.62 + 1.55i, -1.03 - 1.31i, 0.87 + 0.50i, \\ 0.87 + 0.50i, (3)10^{-10} - 1.00i, -0.62 + 1.55i, -1.03 - 1.31i, 1.65 - .24i, -0.87 + 0.50i, \\ -0.87 + 0.50i, 0.87 + 0.50i, -1.03 - 1.31i, 1.65 - 0.24i, -0.62 + 1.55i, (2)10^{-10} - 1.00i, \\ 0.37 - 0.47i, -0.60 - 0.09i, 0.87 + 0.50i, -0.87 + 0.50i, (2)10^{-10} - 1.00i, 0.22 + 0.56i \end{bmatrix}.$$

Selecting the values corresponding to $s_1s_2 = -p = -i$, we obtain 6 pairs of (s_1, s_2) values.

$$(s_1, s_2) = [(1.29 - 0.09i, 0.06 - 0.77i), (-0.56 + 1.16i, -0.70 + 0.34i), (-0.72 - 1.07i, 0.64 + 0.43i), (0.06 - 0.77i, 1.29 - 0.09i), (-0.70 + 0.33i, -0.56 + 1.16i), (0.64 + 0.43i, -0.72 - 1.07i)].$$

Adding the pairs together, we obtain each of the 3 solutions twice, because of the obvious symmetry.

4.2 Using one value from set

We have, for this case, to evaluate

$$s_1 = \left(1 + (1-i)^{1/2}\right)^{1/3} = \left(1 + (1.10 - 0.46i)e^{i\pi k_1}\right)^{1/3}$$

where $k_1 = 0, 1$. There does not seem to be any way to proceed further with this calculation except by substituting values for k_1 . Therefore the approach becomes equivalent to that of the previous section.

4.3 Using principal values

Any of the current computational systems can evaluate the fractional powers as principal values. Thus,

$$\begin{array}{rcl} s_1 & = & \sqrt[3]{1+\sqrt{1-i}} = 1.29 - 0.09i \; , & s_2 = 0.64 + 0.43i \; , \\ y_1 & = & 1.93 + 0.34i \; , & y_2 = -0.51 + 0.39i \; , & y_3 = -1.42 - 0.73i \; , \\ Y_1 & = & 1.34 - 0.86i \; , & Y_2 = -1.26 + 1.50i \; , & Y_3 = -0.08 - 0.63i \; . \end{array}$$

The values Y_1, Y_2, Y_3 are correct and the others are wrong. Notice that all the values $y_1, y_2, y_3, Y_1, Y_2, Y_3$ appear in the set (15).

4.4 Using the surd function

Maple can evaluate the formulae using surd. We have

$$S_1 = \operatorname{surd}(1 + \operatorname{surd}(1 - i, 2), 3) = 1.29 - 0.09i , \quad S_2 = \operatorname{surd}(1 - \operatorname{surd}(1 - i, 2), 3) = -0.70 + 0.34i ,$$

$$y_1 = 0.59 + 0.25i , \quad y_2 = 0.08 + 1.59i , \quad y_3 = -0.67 - 1.84i ,$$

$$Y_1 = 1.34 - 0.86i , \quad Y_2 = -1.26 + 1.50i , \quad Y_3 = -0.08 - 0.63i .$$

Notice that Y_1, Y_2, Y_3 are again correct, and again the y_k and Y_k appear in the set (15).

5 Commentary on the solutions

Some observations can now be made about the above calculations, keeping in mind our primary focus: the question of which of the definitions $\S 3.1 - \S 3.4$ is best for a computer algebra system.

5.1 Using sets of values

From the point of view of implementing this approach in a CAS, the manipulations of the lists of values are not difficult. An obvious drawback is one of efficiency. Although we knew from the start that only 3 solutions existed, we still ended up testing 21 candidate solutions. A potential drawback that is not illustrated by the example concerns the selection of correct answers. The correct solutions were easily identified here, but identifying zero from floating-point data can potentially be difficult.

The numerical example also illustrates the difficulties inherent in trying to implement this definition symbolically. We see that the sets for s_1 and s_2 are equal, and so we have

$$s_1 = \left\{ \left(q + \left\{ (q^2 + p^3)^{\frac{1}{2}} \right\} \right)^{\frac{1}{3}} \right\} = s_2 = \left\{ \left(q - \left\{ (q^2 + p^3)^{\frac{1}{2}} \right\} \right)^{\frac{1}{3}} \right\} .$$

This is a consequence of the simpler statement $\{x^{1/2}\}=-\{x^{1/2}\}$. A symbolic difficulty following from this is the statement

$$y = s_1 + s_2 = s_1 + s_1 \neq 2s_1$$
.

This also reflects a simpler statement, namely that $\{1,2\} + \{1,2\} = \{2,3,4\}$, but $2\{1,2\} = \{2,4\}$. Perhaps an even greater problem is posed by the fact that the statement x = y does not imply x - y = 0. Clearly these difficulties are just the tip of an iceberg of problems connected with the construction of a genuine algebra of multivalued functions. The difficulties are reminiscent of those faced in interval arithmetic, see for example [18, 20].

In conclusion, this approach of selecting from a set of values works satisfactorily, but not efficiently, for formula evaluation. However, a new algebra would have to be discovered and implemented, before a CAS could consistently transform symbolic expressions.

5.2 Using one value from set

Although this definition has been advocated by such influential people as Carathéodory [8, 4], the example shows that it is not useful for computation. It may be useful for admiring the beauty of equations such as $\ln(z_1z_2) = \ln z_1 + \ln z_2$, but not for computation.

5.3 Using principal values

The advantage of principal values is one of efficiency: three roots were required, and 3 were computed. The drawback of principal values is the difficulty of deriving correct formulae. Indeed, the cubic illustrates this. One reason for choosing the cubic equation as the example used here was precisely the fact that, for many years, computer-algebra developers and others did not realize that the traditional formulae could not be used in combination with principal-value powers. As mentioned in the introduction, the problems arising when working with principal values have become an identifiable research area.

5.4 Using surd

The fact that the computations with surd arrived at correct solutions is not a coincidence. Derivations of the Cardano formulae usually point out that any cube root can be used to obtain correct roots, provided it is handled correctly in the resulting formulae. The point is that once a uniquely defined fractional power has been defined, be it principal value or surd, by a CAS or reference book, then it is up to the CAS or book to provide formulae that work with that definition. Thus it would be possible for two different books, using different cube roots, to publish different formulae for cubic roots and each to be correct. Errors would only arise if the formulae from one source were used with the definitions from the other.

6 Riemann surfaces

There is at least one other way of computing with fractional powers, but we have not discussed it here. In conversations at conferences, one sometimes hears the assertion that Riemann surfaces should be used for fractional power computations. We agree that Riemann surfaces form a beautiful theory, and that they are an attractive way to think about multivalued functions. However, what has not been demonstrated, to our knowledge, is the fact that they can be computational. Perhaps some reader can contribute a demonstration of the way in which the theory of Riemann surfaces can be used to solve the example problem discussed here.

7 Concluding remarks

We think that we have demonstrated that principal-valued functions are the best ones for a computer algebra system, and indeed for most mathematical computations, but we hope that this is not the end of the discussion. It would be useful, for example, to have more problems with which the different approaches could be compared. For the present example problem, principal-value functions gave the best solution, but we are open to the possibility that there are other problems for which this conclusion is not correct. Certainly the surd function was introduced into MAPLE so that users could use it, not to prove that it was useless. This is a moot point, however, since we must ask how many mathematicians, even MAPLE users, know of the function. We would like to hear about other system perspectives on the problem. Did discussions similar to this one take place during the development of other systems, such as (in chronological order) MACSYMA, DERIVE and MATHEMATICA? How should these ideas be propagated to the rest of the mathematical world?

We see a connection between the present discussion and Buchberger's advocacy of mathematical research in the computer age [6, 7]. In both cases, the algorithmic aspect of mathematics, whether old mathematics or new, is being raised to a higher level — let us call it the algorismation of mathematics¹.

We close with a few memories of the MAPLE discussions and the reasons advanced for preferring the multivalued interpretation of functions.

- Stupid Maple. Some developers were concerned that if MAPLE refused to honour a request to expand ln(AB) into ln A + ln B, then the users would dismiss the product as being ignorant.
- Ugly Maple. Some developers pined for the good old days when they could enjoy the simplicity of

$$\left(\left(\left(\left((z^2)^{\frac{1}{2}} \right)^3 \right)^{\frac{1}{3}} \right)^4 \right)^{\frac{1}{4}} \to z .$$

• Unresponsive Maple. Sometimes one wants to force a transformation such as $\ln(AB) \to \ln A + \ln B$, because it might prove to be correct later. Equation solving is a typical situation. Sometimes one wants to force the transformation because it is wrong. Rectifying transformations are an example [16].

These objections were met by a variety of mechanisms, such as providing facilities for recording the assumed domains of variables.

¹In [7], Buchberger's German term was translated as *algorithmization*. However, this word is a mouthful to say. The neologism offered here is easier to pronounce, and in addition carries echoes of *automation* as well as being closer to the Persian etymological source of the word algorithm. Obviously, there is a verb *algorismate* waiting to be used.

Appendix: Properties of Cardano formulae

Although the Cardano formulae were introduced as an example for testing multivalued definitions, and were not the main subject of this article, several reviewers were stimulated to re-examine the properties of (2)–(10). Since, to some extent, the main discussion requires that the reader have confidence in the formulae, we record some of the reviewers' comments and questions here.

The formulae look the same. One of the problems of working with principal-valued functions in the complex plane is the need to 'unlearn' some of our reflexive use of transformations. As the numerical examples show, the forms are not equivalent.

The formulae are discontinuous. Assuming principal-valued functions, one finds that the Cardano expressions are discontinuous, even though the roots of the polynomial vary continuously with the coefficients. The observation is correct, but it does not invalidate the correctness of the expressions.

Are the expressions always correct? For the purposes of this paper, we are accepting that MAPLE and MATHEMATICA are using expressions that are correct for principal-branch functions. A full discussion of the correctness and the merits of the different forms of the Cardano formulae must wait for a separate paper.

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