COMPUTATIONAL METHODS IN SCIENCE AND TECHNOLOGY **11(1)**, 73-79 (2005)

Poisson's ratio of anisotropic systems

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(Rec. 30 May 2005)

Abstract: The Poisson's ratio of anisotropic materials depends, in general, both on a "longitudinal" direction along which the stress is changed and on a "transverse" direction in which the transverse deformation is measured. For cubic media there exist "longitudinal" directions, parallel to the 4-fold and 3-fold axes, for which the Poisson's ratio does not depend on the "transverse" direction. Depending on the tensor of elastic compliances (or elastic constants), crystals of cubic symmetry can exhibit negative Poisson's ratio in both these directions (they are called *strongly auxetics*), in one of them (*i.e.* either along the 4-fold axis or along the 3-fold one; they are called *partially auxetic*) or in none of them. For crystals exhibiting 3-fold symmetry axis the Poisson's ratio along this axis does not depend on the "transverse" direction. For other "longitudinal" directions the Poisson's ratio depends, in general, on the "transverse" direction. The Poisson's ratio averaged with respect to the "transverse" direction depends only on the "longitudinal" direction and can be conveniently presented graphically. As an example the *f.c.c.* hard sphere crystal is considered. It is shown that the average (with respect to "transverse" direction) Poisson's ratio of the hard sphere crystal is positive for all "longitudinal" directions. One should add, however, that there exist directions for which the (not averaged) Poisson's ratio of hard spheres is negative.

Key words: elastic properties of crystals of cubic symmetry, negative Poisson's ratio, auxetics

1. INTRODUCTION

Poisson's ratio is a negative ratio of transverse dimension change to longitudinal dimension change of a body when an infinitesimal change of a stress acting along the longitudinal direction occurs whereas the other stress components remain unchanged [1]. Typically the Poisson's ratio of isotropic materials is positive, *i.e.* common materials shrink transversely when stretched [1]. In 1987 Lakes manufactured foams which show negative Poisson's ratio [2]. A recent review of negative Poisson's ratio materials, known also as *anti-rubber* [3], *dilational materials* [4] or *auxetics* [5], can be found in [6]. In this note we briefly discuss Poisson's ratio of anisotropic media [7, 8], illustrating the discussion by systems of cubic symmetry.

2. THE POISSON'S RATIO OF ANISOTROPIC MEDIA

When the stress component, σ_{nn}, in the (longitudinal) direction **n** is changed by $\Delta\sigma_{nn}$ then the strain component in the same direction, ε_{nn}, and the strain component, ε_{mm}, in the (transverse) direction **m** perpendicular to **n** are changed by [1]

$$\Delta\varepsilon_{nn} = S_{nnnn}\,\Delta\sigma_{nn}\,, \tag{1a}$$

$$\Delta\varepsilon_{mm} = S_{mmnn}\,\Delta\sigma_{nn}\,, \tag{1b}$$

where S_{nnnn} and S_{mmnn} are the components of the compliance tensor. Thus, the Poisson's ratio for the longitudinal direction **n** and the transverse direction **m** can be written as

$$\nu_{nm} = -\frac{\Delta\varepsilon_{mm}}{\Delta\varepsilon_{nn}} = -\frac{S_{mmnn}}{S_{nnn}}. \tag{2}$$

Using elementary tensor analysis one can write

$$\nu_{nm} = -\frac{\sum_i\sum_j\sum_k\sum_l m_i m_j n_k n_l S_{ijkl}}{\sum_i\sum_j\sum_k\sum_l n_i n_j n_k n_l S_{ijkl}}, \tag{3}$$

what can be easily calculated when the components, S_{ijkl}, of the compliance tensor are known. The latter one is the inverse of the tensor of elastic constants [9]

$$\sum_p\sum_r S_{ijpr} B_{prkl} = \frac{\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}}{2}, \tag{4}$$

where δ_{ij} is the Kronecker delta and B_{ijkl} are the components of the tensor of elastic constants at the stress $\boldsymbol{\sigma}$. They can be easily related to the elastic constants in the free energy expansion with respect to strain [10].

The direction **n** will be further represented by a pair of angles (φ, θ); θ measures the angle between the **z** axis and **n** whereas φ is the angle between the **x** axis and the projection of the direction **n** on the *xy* plane. (When **n** is parallel or anti-parallel to **z**, *i.e*. when $\theta = 0$ or $\theta = \pi$ then φ can be any number between 0 and 2π.) The direction **m** (perpendicular to **n**) will be represented by a single angle α between the line being the cross section of the plane xy and such a plane perpendicular to **n** which contains the centre of the coordinate system. (When $\theta = 0$ or $\theta = \pi$ then α is the angle between the **x** axis and **m**.)

Thus, in general, the Poisson's ratio given by (3) is a function of three angles

$$\nu_{nm} = \nu(\varphi, \theta, \alpha) \,. \tag{5}$$

Averaging with respect to all the transverse directions (*i.e*. averaging by α) one obtains

$$\nu_P = \nu_P(\varphi,\theta) = \frac{\int \nu(\varphi,\theta,\alpha)d\alpha}{\int d\alpha}, \tag{6}$$

what is convenient for graphical representation.

In the following sections we illustrate the above considerations in the case of cubic media.

3. POISSON'S RATIO OF CUBIC MEDIA

Stability conditions for cubic media can be written in the form

$$\begin{gathered} S_{11} > 0, \quad S_{44} > 0 \\ S_{11} > S_{12} > -\frac{S_{11}}{2}, \end{gathered} \tag{7}$$

where the Voigt notation ($S_{11} = S_{xxxx}$, $S_{12} = S_{xxyy}$, $S_{44} = 4S_{xyxy}$) is used for the compliances of a crystal which 4-fould axes form the reference system.

If one introduces the variables r_{12} and r_{44} defined as

$$\begin{gathered} 1 > r_{12} = \frac{S_{12}}{S_{11}} > -\frac{1}{2}, \\ r_{44} = \frac{S_{44}}{S_{11}} > 0 \end{gathered} \tag{8}$$

then the Poisson's ratio averaged with respect to transverse direction can be written in the form

$$\nu_P(\varphi,\theta) = -\frac{Ar_{12} + B(r_{44} - 2)}{16[C + D(2r_{12} + r_{44})]}, \tag{9}$$

where

$$A = 2\left[53 + 4\cos(2\theta) + 7\cos(4\theta) + 8\cos(4\varphi)\sin^4\theta\right], \tag{10a}$$

$$B = -11 + 4\cos(2\theta) + 7\cos(4\theta) + 8\cos(4\varphi)\sin^4\theta, \tag{10b}$$

$$C = 8\cos^4\theta + 6\sin^4\theta + 2\cos(4\varphi)\sin^4\theta, \tag{10c}$$

$$D = 2[\sin^2(2\theta) + \sin^4\theta \sin^2(2\varphi)]. \tag{10d}$$

Analysis of the first derivative of $\nu_P(\varphi, \theta)$ with respect to φ, θ shows that it is zero in the high symmetry directions [100], [111], [110]. For these (extreme or saddle-point) directions, the average Poisson's ratio can be written as

$$\nu_P(100) = -r_{12}\,, \tag{11a}$$

$$\nu_P(111) = -\frac{1 + 2r_{12} - r_{44}/2}{1 + 2r_{12} + r_{44}}, \tag{11b}$$

$$\nu_P(110) = -\frac{1 + 3r_{12} - r_{44}/2}{2 + 2r_{12} + r_{44}}. \tag{11c}$$

It is worth to stress that in [100] and [111] directions $\nu_P(\varphi, \theta) = \nu(\varphi, \theta, \alpha)$, *i.e*. $\nu(\varphi, \theta, \alpha)$ does not depend on α.

To illustrate the behaviour of the Poisson's ratio, instead of using r_{44} which changes between 0 and infinity, a variable x which varies between 0 and 2 will be used

$$x = r_{44}, \qquad \text{if} \quad r_{44} \le 1, \tag{12a}$$

$$x = 2 - 1/r_{12}\,, \quad \text{if} \quad r_{44} > 1 \tag{12b}$$

and (to simplify notation) r_{12} will be replaced by y.

In Fig. 1 the average (with respect to "transverse" directions) Poisson's ratio, ν_P, is shown as a function of x and y in the high symmetry directions. It can be seen that in each of those directions the average Poisson's ratio can be positive (and lower than ½) or negative (and higher than −1). The sets of (x, y) points for which the average Poisson's ratios are equal to zero form curves which are presented in Fig. 2. It can be seen there that the curve corresponding to the direction [110] is always between the other two curves. This means that when one changes y keeping x fixed, the sign of the average Poisson's ratio in the [110] direction is never changed as the first or the last one of these tree directions. Thus, there are only three possibilities for cubic systems:

(1) The average Poisson's ratio is positive both in [100] and [111] directions. If so, the average Poisson's ratio is positive in any direction.
(2) The average Poisson's ratio is positive in one of [100] and [111] directions and negative in the other one. Such a system will be further referred to as *partially auxetic*.
(3) The average Poisson's ratio is negative both in [100] and [111] directions. The average Poisson's ratio must be then negative in any direction. Such a system, further referred to as *strongly auxetic.*

It is obvious that the mean value, $<\nu_P>$, of the Poisson's ratio (averaged with respect to *both* "longitudinal" and "transverse" directions) is negative for strongly auxetic systems. For axial auxetics the mean can be negative or

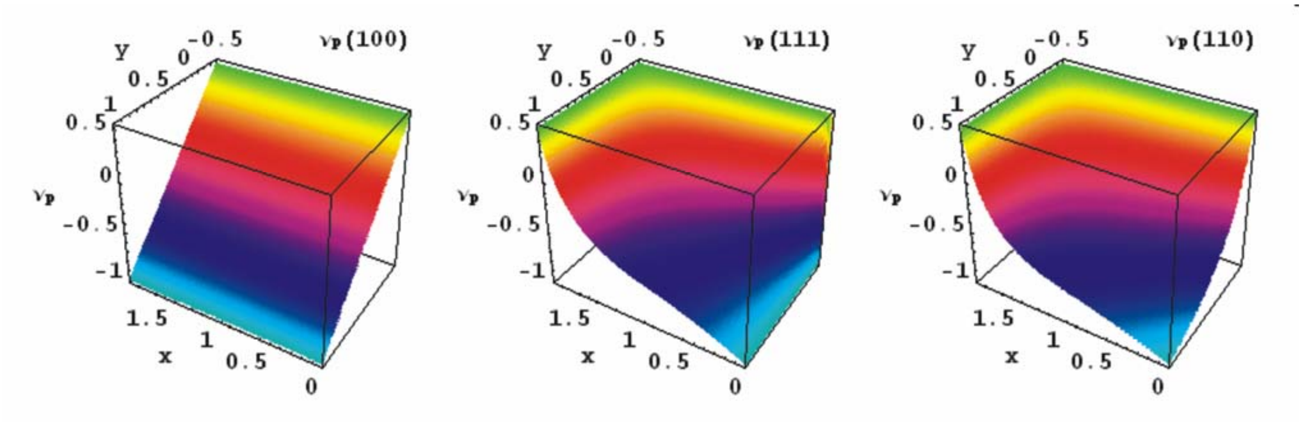

Fig. 1. The average Poisson's ratios in the high symmetry directions
as functions of the parameters x and y defined in (12)

positive. Systems with the negative mean value will be further referred to as *effectivelly auxetic*.

In Fig. 3 the x, y regions corresponding to various kinds of cubic auxetics are shown. As expected, the set representing effectively auxetic systems contains the set representing strongly auxetic systems.

The two-angle function, $\nu_P(\varphi, \theta)$, can be represented in the spherical coordinates as a surface which distance from the coordinate centre in the "longitudinal" direction $\mathbf{n}(\varphi, \theta)$ corresponds to the amplitude of the Poisson's ratio. To avoid problems with interpretation of the sign of ν_P it is convenient to show its positive and negative values in two separated plots: in the left one the positive amplitudes are shown, whereas in the right one the absolute values of the negative amplitudes are presented. In Fig. 4 some examples of such plots are shown for some values of x, y.

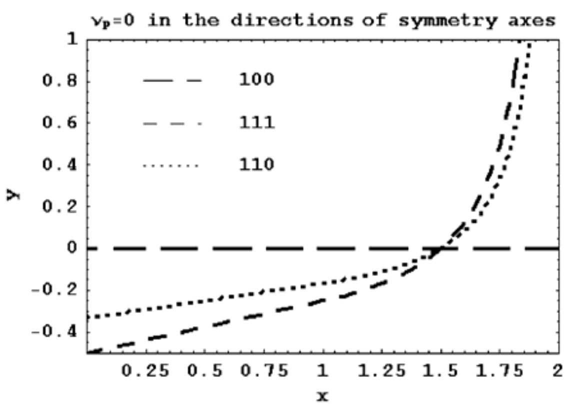

Fig. 2. The x, y curves for which the averaged (with respect to transverse direction) Poisson's ratios change signs in the (longitudinal) high symmetry directions

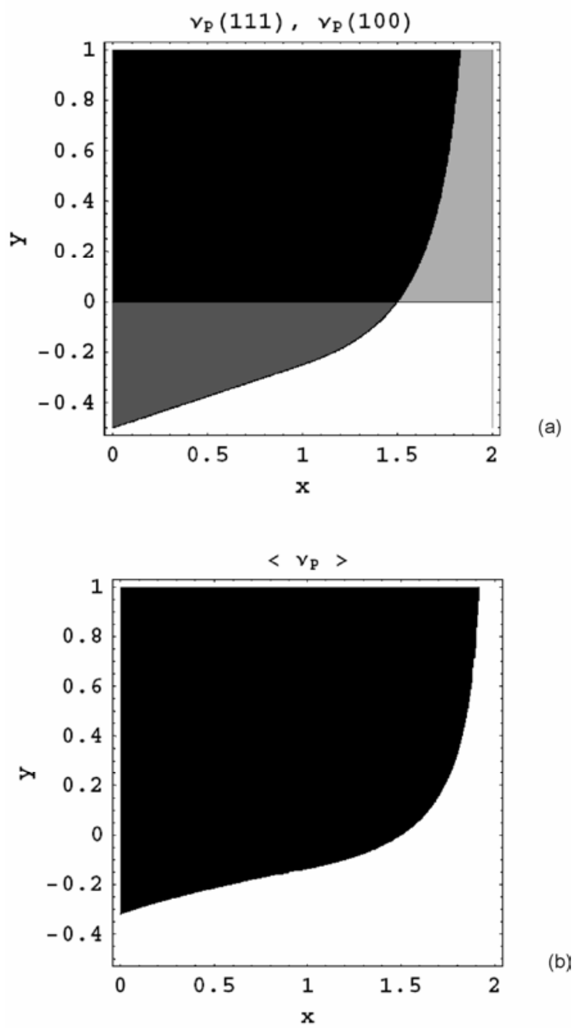

Fig. 3. (a) The x, y range for strongly auxetic (black) and partially auxetic (gray) materials. (b) The x, y range for effectively auxetic systems (black)

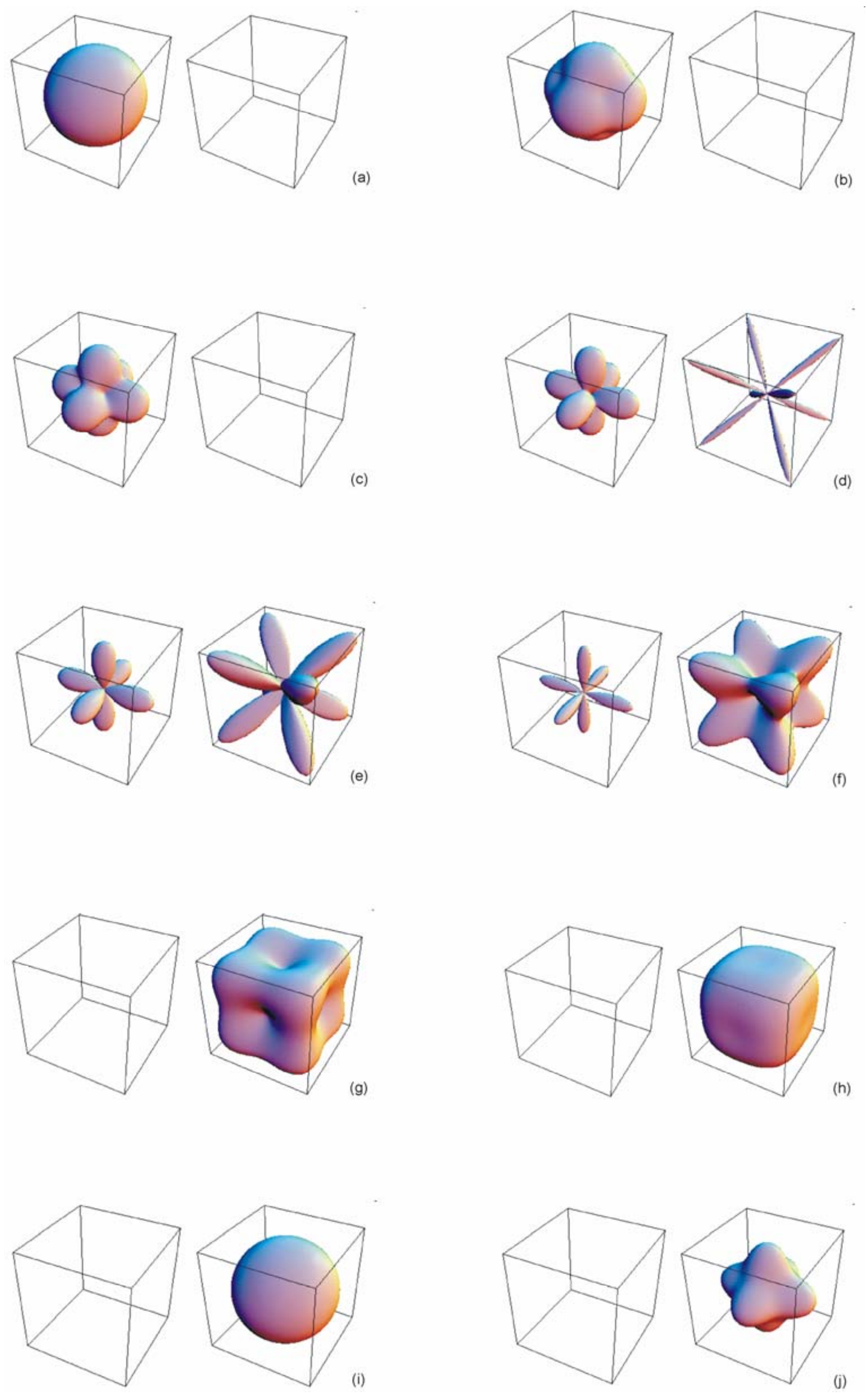

Fig. 4. The average (with respect to transverse direction) Poisson's ratio in the spherical coordinate system and the mean values, $\langle\nu_P\rangle$, of the Poisson's ratio. In each case $x = 1$. (a) $y = -0.5$, $\langle\nu_P\rangle = 0.5$; (b) $y = -0.44$, $\langle\nu_P\rangle = 0.397$; (c) $y = -0.34$, $\langle\nu_P\rangle = 0.248$; (d) $y = -0.24$, $\langle\nu_P\rangle = 0.119$; (e) $y = -0.15$, $\langle\nu_P\rangle = 0.016$; (f) $y = -0.05$, $\langle\nu_P\rangle = -0.085$; (g) $y = 0.15$, $\langle\nu_P\rangle = -0.259$; (h) $y = 0.35$, $\langle\nu_P\rangle = -0.405$; (i) $y = 0.5$, $\langle\nu_P\rangle = -0.5$; (j) $y = 1.0$, $\langle\nu_P\rangle = 0.757$. For simplicity, only shapes of the Poisson's ratio are shown and no amplitudes are presented

4. POISSON'S RATIO OF HARD SPHERES

The hard sphere system is the simplest model exhibiting the melting transition. The interactions in the system are purely geometric ones, *i.e.* the spheres interact through the hard potential which is infinite when any overlap occurs in the system and zero otherwise.

There was a debate in eighties of the last century if the hard sphere system shows negative Poisson's ratio. The debate was initiated by a density functional approach proposed by Jaric and Mohanty [11] who claimed that the Poisson's ratio of the *f.c.c.* crystal of hard spheres is negative. Frenkel and Ladd showed, however, that that the Poisson's ratio of hard spheres is positive [12]. In both those papers only the [100] direction was discussed.

In Fig. 5 the average (with respect to transverse direction) Poisson's ratio is shown for all possible longitudinal directions for the *f.c.c.* crystal of hard spheres in the close packing limit. The elastic constants from which this dependence was determined were obtained recently in Ref. [13]. It can be seen that the average Poisson's ratio of hard spheres is positive for any longitudinal direction and the Poisson's ratio strongly depends on the direction.

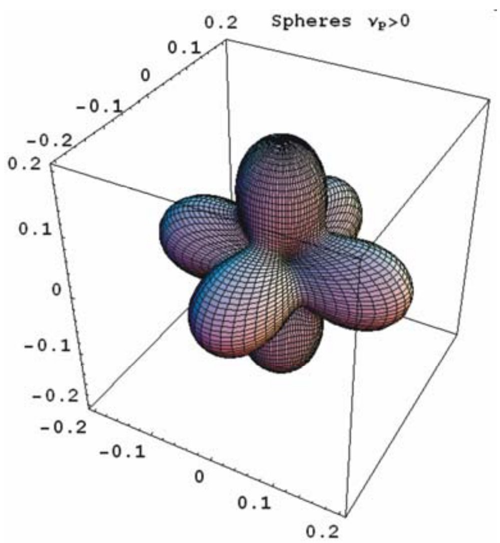

Fig. 5. The average (with respect to transverse direction) Poisson's ratio for hard spheres in the close packing limit

In Fig. 6 the α-dependence of the Poisson's ratio is drawn for the "longitudinal" direction [110]. It is easy to notice that in the transverse direction [1$\underline{1}$0] the Poisson's ratio is negative for the hard sphere system. A general theoretical basis concerning possibility of finding a negative Poisson's ratio in *f.c.c.* cubic crystals has been done already in 1977 by Milstein and Huang [14]. More recently, Baughman and co-workers have shown that the Poisson's ratio is those directions is negative for many

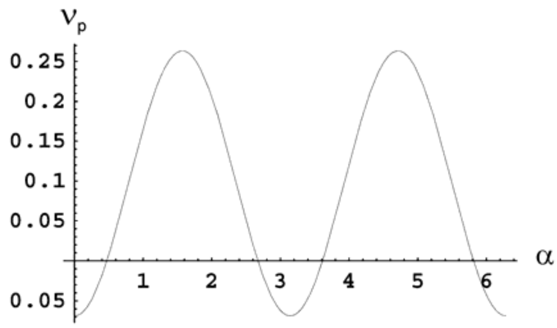

Fig. 6. The α-dependence of the Poisson's ratio in the "longitudinal" direction [110] for the f.c.c. crystal of hard spheres in the close packing limit

cubic crystals [15]. It is also worth to add that for the same "longitudinal" and "transverse" directions Runge and Chester have obtained negative Poisson's ratio of amplitude −0.054 +/− 0.009 near melting [16].

5. SUMMARY AND CONCLUSIONS

The Poisson's ratio, averaged with respect to transverse direction, has been presented for anisotropic media. The behaviour of this quantity has been illustrated for cubic crystals, in general, and for the hard spheres, in particular.

The averaged Poisson's ratio can play the role of a convenient function characterizing elastic properties of anisotropic systems.

Acknowledgments

This work was supported by the (Polish) State Committee for Scientific Research grant 4T11F01023. Part of the computations was performed at the Poznań Networking and Supercomputing Center.

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