

ON MACROSCOPIC ELASTIC PROPERTIES OF ISOTROPIC DISCRETE SYSTEMS: EFFECT OF TESSELLATION GEOMETRY

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Abstract. Discrete mesoscale models of heterogeneous materials attracts increased attention thanks to their robustness, relative simplicity and direct representation of complex phenomena taking place during fracture initiation and propagation. Their major drawback is limitations imposed on macroscopic Poisson's ratio, thus they can be used only for material with low Poisson's ratio.

The contribution develops analytical formulas for estimation of macroscopic Poisson's ratio of two dimensional isotropic discrete systems where artificial distribution of angle between contact vectors and contact facets is assumed. The analytical formulas unfortunately lead to conclusion that the Poisson's ratio cannot be increased by model geometrical changes. The widest range of possible Poisson's ratio is obtained for perpendicular contact vector and contact facet, i.e. for the models used in most of the literature on this topic.

1 INTRODUCTION

There is large demand in research and industry for reliable models capable to predict behavior of heterogeneous cohesive materials. The contribution is focused on concrete, material composed of mineral aggregates and binding matrix. One particular group of models, known as discrete models [3,7], is studied. The discrete models, thanks to assumption of discontinuous displacement field, easily capture concrete fracture behavior, but brings difficulties in elastic regime.

Discrete mechanical models are often formulated with vectorial constitutive law assuming linear relation between stress and strain both in normal and tangential direction. It is well known that Poisson ratio of such systems is limited within range from -1 to 1/4 for 3D systems, from -1 to 1/3 for 2D plane stress simplifications and from negative infinity to 1/4 for 2D

plane strain simplifications. These limits, when compared to real materials with greater Poisson's ratio, challenge many researchers.

Recently, two remedies providing full range of Poisson's ratio in discrete systems were presented. The first one [1, 2] introduces artificial auxiliary stresses within iterative loop to achieve elastically homogeneous system of arbitrary Poisson's ratio. The second remedy [5] is based on splitting the strains into volumetric and deviatoric part. The stress oscillations caused by heterogeneity of the material are unfortunately smeared out in both cases. Such models are therefore not convenient for studying highly heterogeneous structures at mesoscale.

It has been shown that three fundamental assumptions are needed to derive the Poisson's ratio limits, namely the isotropy of geometrical structure, space tessellation into discrete

units without any voids or overlaps and perpendicularity between contact facets and contact vectors [6]. The third assumption is relaxed here and implications are studied. It is shown by analytical derivations in two dimensions (using strong assumptions about rotations and translations in the model according to [8]) that the modification of the angle between contact normal and contact length vector results in changes in Poisson's ratio. The paper unfortunately proves that geometrical changes leads only to shrinking of the interval of achievable Poisson's ratios.

Equations are derived based on equivalence of virtual work arising in the discrete system and continuum subjected to equal straining. The Boltzmann continuum is used, therefore the stress tensor must be symmetric (Boltzmann axiom). However, the discrete system yields non-symmetric stress tensor, as it is rather discrete instance of polar (Cosserat) continua [9]. The symmetrization of the tensor of elastic constants from the discrete model is employed to establish the equivalence.

2 NORMAL AND CONTACT VECTORS

Two dimensional domain is divided into rigid bodies, each of them have degrees of freedom associated with translations and rotations of some inner node, \mathbf{x}_a . The contact between two nodes \mathbf{x}_a and \mathbf{x}_b is provided by mechanical element with facet area A , length l , unit normal vector \mathbf{n} and contact vector $\mathbf{t} = (\mathbf{x}_b - \mathbf{x}_a) / \|\mathbf{x}_b - \mathbf{x}_a\|$. The situation is sketched in Fig. 1a.

We assume that the system has no directional bias, therefore all normal directions share the same probability of occurrence. The vector \mathbf{n} is here defined in Cartesian coordinate system by angles ξ

$$\mathbf{n} = (\cos \xi, \sin \xi) \quad (1)$$

ξ represents angle between x axis and the normal and covers uniformly the solid angle.

$$f_\xi(\xi) = \begin{cases} \frac{1}{2\pi} & \text{for } \xi \in (0, 2\pi) \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

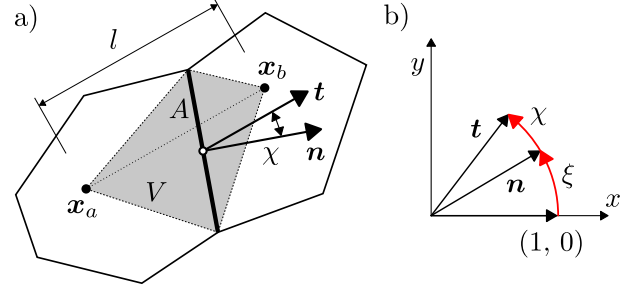


Figure 1: a) Two dimensional rigid bodies in contact. The shaded area represents single mechanical element with normal vector \mathbf{n} , contact vector \mathbf{t} , area A , length l and volume V ; b) normal and contact vector.

The second fundamental vector governing behavior of the contact is the contact vector \mathbf{t} . It is defined relatively to normal vector \mathbf{n} by angles χ - see Fig. 1b. To ensure isotropic, directionally unbiased 2D structure, χ must have probability distribution symmetric around zero. For sake of simplicity, it will be assumed here that χ has uniform distribution in range $(-\gamma, \gamma)$.

$$f_\chi(\chi) = \begin{cases} \frac{1}{2\gamma} & \text{for } \theta \in (-\gamma, \gamma) \\ 0 & \text{otherwise} \end{cases} \quad (3)$$

Let us define rotation matrix

$$\mathbf{R}(\chi) = \begin{bmatrix} \cos \chi & -\sin \chi \\ \sin \chi & \cos \chi \end{bmatrix} \quad (4)$$

that provides the following relation between \mathbf{n} and \mathbf{t}

$$\mathbf{t} = \mathbf{R} \cdot \mathbf{n} \quad (5)$$

The cosine of angle χ between \mathbf{n} and \mathbf{t} can be calculated using the rotation matrix

$$\cos \chi = \mathbf{n} \cdot \mathbf{t} = \mathbf{n} \cdot \mathbf{R} \cdot \mathbf{n} = \mathbf{R} : \mathbf{N} \quad (6)$$

where the second order tensor \mathbf{N} is according to [8] defined as $\mathbf{N} = \mathbf{n} \otimes \mathbf{n}$. Based on assumption of no gaps or overlapping between rigid bodies of the model, the total volume is summation over volume of individual mechanical elements

$$V = \sum_e V_e = \sum_e \cos \chi_e \frac{A_e l_e}{N_{\text{dim}}} = \sum_e \mathbf{R}_e : \mathbf{N}_e \frac{A_e l_e}{2} \quad (7)$$

Note that volume of individual element is negative whenever $|\chi| > \pi/2$.

3 VIRTUAL WORK EQUIVALENCE

The derivation is based on assumption that when the discrete system is subjected to constant strain $\boldsymbol{\varepsilon}$, all the rotations are zeros and differences in translations are dictated by differences in position

$$\boldsymbol{\varphi} = 0 \quad \mathbf{u}_b - \mathbf{u}_a = \boldsymbol{\varepsilon} \cdot (\mathbf{x}_b - \mathbf{x}_a) \quad (8)$$

This assumption is taken according to [8]. The displacement jump on contact between cells a and b is then given by

$$\boldsymbol{\Delta} = \mathbf{u}_b - \mathbf{u}_a = l\boldsymbol{\varepsilon} \cdot \mathbf{t} \quad (9)$$

where l and \mathbf{t} are length and contact vector belonging to element connecting bodies a and b . The normal and shear strain and stress directly follow

$$e_N = \frac{\mathbf{n} \cdot \boldsymbol{\Delta}}{l} = \mathbf{n} \cdot \boldsymbol{\varepsilon} \cdot \mathbf{t} \quad (10)$$

$$e_T = \frac{\boldsymbol{\Delta}}{l} - e_N \mathbf{n} = \boldsymbol{\varepsilon} \cdot \mathbf{t} - (\mathbf{n} \cdot \boldsymbol{\varepsilon} \cdot \mathbf{t}) \mathbf{n} \quad (11)$$

The stresses are defined using two material parameters constant in the whole domain: E_0 is the normal stiffness coefficient and α is the tangential/normal stiffness ratio.

$$s_N = E_0 e_N \quad \mathbf{s}_T = E_0 \alpha e_T \quad (12)$$

The virtual work of single element obtained by integration of product of constant stress and displacement jump over the contact area A yields

$$\delta W = Al (s_N \delta e_N + \mathbf{s}_T \cdot \delta \mathbf{e}_T) \quad (13)$$

To simplify the notation, we introduce operation transposition T_{ij} on arbitrary tensor \mathbf{A} of sufficient order by swapping indices i and j .

$$A_{\dots i \dots j \dots}^{T_{ij}} = A_{\dots j \dots i \dots} \quad (14)$$

According to [8], let us now define two additional tensors: the fourth order tensor \mathcal{J}^{vol} and

the third order tensor \mathbf{T} .

$$\mathcal{J}^{\text{vol}} = \frac{\mathbf{1} \otimes \mathbf{1}}{3} \quad (15)$$

$$\mathbf{T} = 3\mathbf{n} \cdot (\mathcal{J}^{\text{vol}})^{T_{13}} - \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \quad (16)$$

where $\mathbf{1}$ is the identity matrix of size 2. Because the symmetry implied by equality $\mathbf{t} = \mathbf{n}$ is no longer present, tensor \mathbf{T} is different from definition in [6, 8].

With the previously defined tensor \mathbf{N} , strains from Eqs. (10) and (11) are rewritten

$$e_N = (\mathbf{N} \cdot \mathbf{R}^{T_{12}}) : \boldsymbol{\varepsilon} \quad (17)$$

$$\mathbf{e}_T = (\mathbf{T} \cdot \mathbf{R}^{T_{12}}) : \boldsymbol{\varepsilon} \quad (18)$$

The virtual work of single element (Eq. (13)) can be rewritten as well.

$$\begin{aligned} \delta W &= Al (s_N \delta e_N + \mathbf{s}_T \cdot \delta \mathbf{e}_T) \\ &= Al E_0 \left([(\mathbf{N} \cdot \mathbf{R}^T) : \boldsymbol{\varepsilon}] [(\mathbf{N} \cdot \mathbf{R}^T) : \delta \boldsymbol{\varepsilon}] \right. \\ &\quad \left. + \alpha [(\mathbf{T} \cdot \mathbf{R}^T) : \boldsymbol{\varepsilon}] \cdot [(\mathbf{T} \cdot \mathbf{R}^T) : \delta \boldsymbol{\varepsilon}] \right) \\ &= Al E_0 \left[\boldsymbol{\varepsilon} : (\mathbf{R} \cdot \mathbf{N} \otimes \mathbf{N} \cdot \mathbf{R}^T)^{T_{12}} : \delta \boldsymbol{\varepsilon} \right. \\ &\quad \left. + \alpha \boldsymbol{\varepsilon} : (\mathbf{R} \cdot \mathbf{T}^{T_{13}} \cdot \mathbf{T} \cdot \mathbf{R}^T) : \delta \boldsymbol{\varepsilon} \right] \\ &= Al E_0 \boldsymbol{\varepsilon} : (\mathcal{N} + \alpha \mathcal{F}) : \delta \boldsymbol{\varepsilon} \quad (19) \end{aligned}$$

where

$$\mathcal{N} = (\mathbf{R} \cdot \mathbf{N} \otimes \mathbf{N} \cdot \mathbf{R}^T)^{T_{12}} \quad (20)$$

$$\mathcal{F} = \mathbf{R} \cdot \mathbf{T}^{T_{13}} \cdot \mathbf{T} \cdot \mathbf{R}^T \quad (21)$$

The total virtual work of the discrete assembly is summation of virtual works from individual elements

$$\begin{aligned} \delta W^{\text{dis}} &= \sum_e \delta W_e \quad (22) \\ &= \sum_e A_e l_e E_0 \boldsymbol{\varepsilon} : (\mathcal{N}_e + \alpha \mathcal{F}_e) : \delta \boldsymbol{\varepsilon} \end{aligned}$$

The virtual work of equally strained elastic isotropic continuum occupying the same volume V is

$$\delta W^{\text{con}} = V \boldsymbol{\sigma} : \delta \boldsymbol{\varepsilon} = V \boldsymbol{\varepsilon} : \mathbf{D} : \delta \boldsymbol{\varepsilon} \quad (23)$$

where \mathbf{D} is fourth order tensor of elastic constants.

The equivalence of the discrete and continuous system implies equality of virtual works

$$\delta W^{\text{dis}} = \delta W^{\text{con}} \quad (24)$$

Substituting Eqs. (22) and (23) into Eq. (24), expression for tensor of elastic constants is derived

$$\mathbf{D} = \left\langle \frac{1}{V} \sum_e A_e l_e E_0 (\mathcal{N}_e + \alpha \mathcal{F}_e) \right\rangle^{\text{SYM}} \quad (25)$$

The symmetrization is necessary because the tensors \mathcal{N} and \mathcal{F} do not have the symmetries required for Boltzmann continuum, which are the major symmetry ($D_{ijkl} = D_{klij}$) and the minor symmetry ($D_{ijkl} = D_{jikl} = D_{ijlk} = D_{jilk}$). Because of the non-symmetric stress tensor in the discrete system, the minor symmetry is violated. The symmetric part is obtained using transposition T_{34} .

$$\langle \bullet \rangle^{\text{SYM}} = \frac{\bullet + \bullet^{T_{34}}}{2} \quad (26)$$

Thanks to assumed statistical independence between normal and contact vector and elemental area and length, the summation can be broken into the following expression

$$\mathbf{D} = \frac{E_0}{V} \langle \mathbf{E}[\mathcal{N}] + \alpha \mathbf{E}[\mathcal{F}] \rangle^{\text{SYM}} \sum_e A_e l_e \quad (27)$$

where $\mathbf{E}[\bullet(\mathbf{x})]$ is the mean value of function \bullet dependent on vector \mathbf{x} with distribution func-

tion $f_{\mathbf{x}}(\mathbf{x})$ defined as

$$\mathbf{E}[\bullet(\mathbf{x})] = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \bullet(\mathbf{x}) f_{\mathbf{x}}(\mathbf{x}) d\mathbf{x} \quad (28)$$

Substituting V from Eq. (7) and utilizing the statistical independence again yields

$$\mathbf{D} = \frac{N_{\text{dim}} E_0}{\mathbf{E}[\mathbf{R} : \mathbf{N}]} \langle \mathbf{E}[\mathcal{N}] + \alpha \mathbf{E}[\mathcal{F}] \rangle^{\text{SYM}} \quad (29)$$

4 INTEGRATION OF EXPECTATIONS

The rotation matrix is dependent only on angle χ , while the normal \mathbf{n} depends only on angle ξ . Let us first calculate all the quantities dependent solely on \mathbf{n} .

$$\mathbf{E}[\mathbf{N}] = \int_0^{2\pi} \mathbf{n} \otimes \mathbf{n} \frac{1}{2\pi} d\xi = \frac{1}{2} \mathbf{1} \quad (30)$$

$$\mathbf{E}[\mathbf{N} \otimes \mathbf{N}] = \int_0^{2\pi} \mathbf{N} \otimes \mathbf{N} \frac{1}{2\pi} d\xi = \frac{1}{4} \mathcal{F} + \frac{3}{8} \mathcal{F}^{\text{vol}} \quad (31)$$

$$\begin{aligned} \mathbf{E}[\mathbf{T}^{T_{13}} \cdot \mathbf{T}] &= \int_0^{2\pi} \mathbf{T}^{T_{13}} \cdot \mathbf{T} \frac{1}{2\pi} d\xi \\ &= \frac{3}{4} \mathcal{F} - \frac{3}{8} \mathcal{F}^{\text{vol}} - \frac{3}{2} (\mathcal{F}^{\text{vol}})^{T_{23}} \end{aligned} \quad (32)$$

where the fourth order tensor $\mathcal{F} = \mathcal{F}_{ijkl} = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})/2$ with $\delta_{ij} \equiv \mathbf{1}$ is the Kronecker delta.

Now, we integrate terms involving both \mathbf{R} and \mathbf{n} .

$$\mathbb{E}[\mathbf{R} : \mathbf{N}] = \frac{1}{2} \int_{-\gamma}^{\gamma} \mathbf{R} : \mathbf{1} \frac{1}{2\gamma} d\chi = \frac{1}{4\gamma} \int_{-\gamma}^{\gamma} 2 \cos \chi d\chi = \frac{\sin \gamma}{\gamma} \quad (33)$$

$$\begin{aligned} \mathbb{E}[\mathcal{N}] &= \int_{-\gamma}^{\gamma} \int_0^{2\pi} \mathcal{N} \frac{1}{2\gamma} \frac{1}{2\pi} d\xi d\chi = \int_{-\gamma}^{\gamma} [\mathbf{R} \cdot \mathbb{E}[\mathbf{N} \otimes \mathbf{N}] \cdot \mathbf{R}^T]^{T_{12}} \frac{1}{2\gamma} d\chi \\ &= \int_{-\gamma}^{\gamma} \left[\mathbf{R} \cdot \left(\frac{1}{4} \mathcal{J} + \frac{3}{8} \mathcal{J}^{\text{vol}} \right) \cdot \mathbf{R}^T \right]^{T_{12}} \frac{1}{2\gamma} d\chi \\ &= \frac{3}{4} (\mathcal{J}^{\text{vol}})^{T_{23}} + \frac{3 \sin 2\gamma}{16\gamma} \left(\mathcal{J}^{\text{vol}} - (\mathcal{J}^{\text{vol}})^{T_{23}} + (\mathcal{J}^{\text{vol}})^{T_{24}} \right) \end{aligned} \quad (34)$$

$$\begin{aligned} \mathbb{E}[\mathcal{J}] &= \int_{-\gamma}^{\gamma} \int_0^{2\pi} \mathcal{J} \frac{1}{2\gamma} \frac{1}{2\pi} d\xi d\chi = \int_{-\gamma}^{\gamma} \mathbf{R} \cdot \mathbb{E}[\mathbf{T}^{T_{13}} \cdot \mathbf{T}] \cdot \mathbf{R}^T \frac{1}{2\gamma} d\chi \\ &= \int_{-\gamma}^{\gamma} \mathbf{R} \cdot \left(\frac{3}{4} \mathcal{J} - \frac{3}{8} \mathcal{J}^{\text{vol}} - \frac{3}{2} (\mathcal{J}^{\text{vol}})^{T_{23}} \right) \cdot \mathbf{R}^T \frac{1}{2\gamma} d\chi \\ &= \frac{3}{4} (\mathcal{J}^{\text{vol}})^{T_{24}} - \frac{3 \sin 2\gamma}{16\gamma} \left(\mathcal{J}^{\text{vol}} + (\mathcal{J}^{\text{vol}})^{T_{23}} - (\mathcal{J}^{\text{vol}})^{T_{24}} \right) \end{aligned} \quad (35)$$

We need only symmetric parts of these expectations. With help of Eq. (26) we derive

$$\langle (\mathcal{J}^{\text{vol}})^{T_{23}} \rangle^{\text{SYM}} = \langle (\mathcal{J}^{\text{vol}})^{T_{24}} \rangle^{\text{SYM}} = \frac{\mathcal{J}}{3} \quad (36)$$

and use it to obtain final the symmetric expectations of tensors

$$\langle \mathbb{E}[\mathcal{N}] \rangle^{\text{SYM}} = \frac{1}{4} \mathcal{J} + \frac{3 \sin 2\gamma}{16\gamma} \mathcal{J}^{\text{vol}} \quad (37)$$

$$\langle \mathbb{E}[\mathcal{J}] \rangle^{\text{SYM}} = \frac{1}{4} \mathcal{J} - \frac{3 \sin 2\gamma}{16\gamma} \mathcal{J}^{\text{vol}} \quad (38)$$

5 MACROSCOPIC ELASTIC PARAMETERS

The mechanical behavior of linearly elastic isotropic solid is determined e.g. by elastic modulus (E) and Poisson's ratio (ν). The tensor of elastic constants is expressed using these variables (upper row will be for plane stress,

bottom row for plane strain hereinafter)

$$\mathbf{D} = \begin{cases} \frac{E}{1+\nu} \mathcal{J} + \frac{3E\nu}{1-\nu^2} \mathcal{J}^{\text{vol}} \\ \frac{E}{1+\nu} \mathcal{J} + \frac{3E\nu}{(1+\nu)(1-2\nu)} \mathcal{J}^{\text{vol}} \end{cases} \quad (39)$$

Equation (29) along with symmetrized expectations (33), (37) and (38) provides

$$\mathbf{D} = E_0 \left[\frac{(1+\alpha)\gamma}{2 \sin \gamma} \mathcal{J} + \frac{3(1-\alpha) \cos \gamma}{4} \mathcal{J}^{\text{vol}} \right] \quad (40)$$

Equality between Eq. (40) and (39) requires equality between respective scalar multipliers of tensors \mathcal{J}^{vol} and \mathcal{J} . Solving the linear sys-

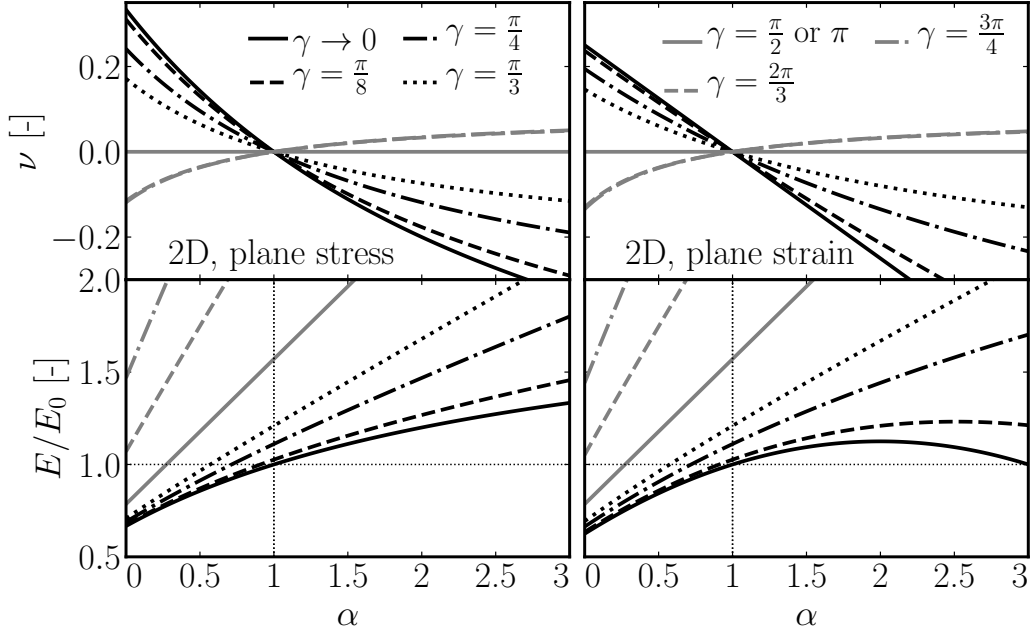


Figure 2: Dependency of macroscopic elastic properties of discrete system with uniformly distributed χ in interval $|\chi| < \gamma$ on tangential/normal stiffness ratio α according to Eqs. (41) and (42).

tem of two equations yields

$$\nu = \begin{cases} \frac{(1-\alpha)\sin 2\gamma}{4(1+\alpha)\gamma + (1-\alpha)\sin 2\gamma} \\ \frac{(1-\alpha)\sin 2\gamma}{4(1+\alpha)\gamma + 2(1-\alpha)\sin 2\gamma} \end{cases} \quad (41)$$

$$E = \begin{cases} E_0 \frac{2(1+\alpha)^2\gamma^2 + (1-\alpha^2)\gamma \sin 2\gamma}{\sin \gamma(4(1+\alpha)\gamma + (1-\alpha)\sin 2\gamma)} \\ E_0 \frac{4(1+\alpha)^2\gamma^2 + 3(1-\alpha^2)\gamma \sin 2\gamma}{\sin \gamma(8(1+\alpha)\gamma + 4(1-\alpha)\sin 2\gamma)} \end{cases} \quad (42)$$

These equations are plotted in Fig. 2.

Decreasing γ towards zero yields relations for discrete system with $\mathbf{n} = \mathbf{t}$ as derived in e.g. [6] under assumption of perpendicularity of contact vector and contact facet. They are also identical to those from microplane theory [4].

$$\lim_{\gamma \rightarrow 0} \nu = \begin{cases} \frac{1-\alpha}{3+\alpha} \\ \frac{1-\alpha}{4} \end{cases} \quad (43)$$

$$\lim_{\gamma \rightarrow 0} E = \begin{cases} E_0 \frac{2+2\alpha}{3+\alpha} \\ E_0 \frac{(1+\alpha)(5-\alpha)}{8} \end{cases} \quad (44)$$

What are the maximum and minimum values of Poisson's ratio that can be achieved? One can differentiate the expression (41) with respect to γ and search for stationary point. Leaving out degenerative case $\alpha = 1$, it reveals local extreme at points $\gamma = 0$ and $\gamma \approx 2.24670$ (solution of $2\gamma = \tan 2\gamma$). Plotting the Poisson's ratio with respect to the limit angle γ (Fig. 3) shows that the maximum range of ν is obtained for $\gamma = 0$, i.e. when the contact vector equals the normal vector. This is the classic solution stated in Eq. (44). Increasing γ up to $\pi/2$ causes shrinking of the interval of achievable Poisson's ratios to zero. Then, the interval opens again with opposite signs; its width maximizes at $\gamma = 2.24670$. The limiting values are obtained at $\alpha = 0$ and $\alpha \rightarrow \infty$ as $(-0.122, 0.098)$ for 2D plane stress, $(-0.139, 0.089)$ for 2D plane strain.

6 Conclusions

We have proven that under assumption (3), one cannot increase the Poisson's ratio limits beyond what is provided by model with $\mathbf{n} = \mathbf{t}$ in Eq. (44). The analysis is now being extended to three dimensions and with consideration of arbitrary distribution function $f_\chi(\chi)$.

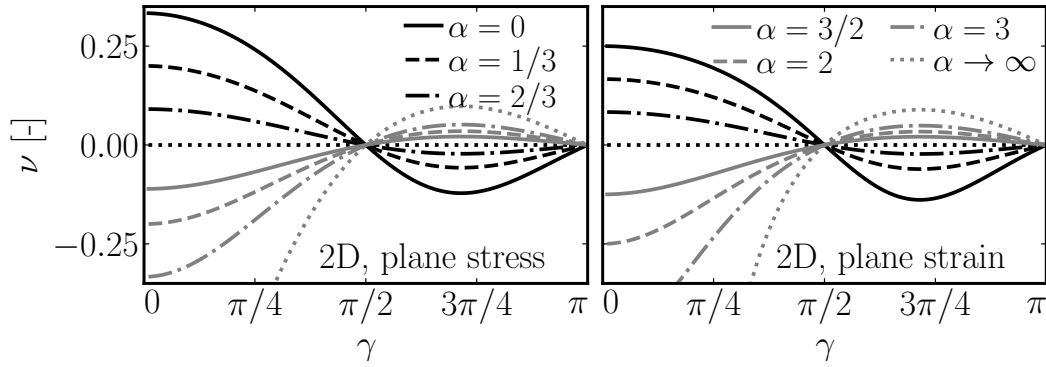


Figure 3: Dependency of macroscopic Poisson's ratio of discrete system with uniformly distributed χ in interval $|\chi| < \gamma$ on the limit γ according to Eq. (41).

It is also planned to numerically verify the results by simulating straining of the discrete system. It is expected that deviations from derived equations will occur due to strong and unrealistic assumption about system degrees of freedom (Eq. (8)). The only case when these assumptions are exactly fulfilled is when $\alpha = 1$ and $n = t$.

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