Anti-plane surface waves in media with surface structures and surface interfaces: Discrete *vs*. continuum model

Victor A. Eremeyev[1] and Basant Lal Sharma[2]

[1]*Gdańsk University of Technology, Poland*; [2]*Indian Institute of Technology Kanpur, India*

Kick-off meeting of the IRP Coss&Vita joint with
Workshop on elastodynamics of microstructured media

October, 17–19, 2019 École des Ponts ParisTech, Champs sur Marne, Amphithéâtre Navier

POLITECHNIKA GDAŃSKA

Outline

The aim of the lecture is

to discuss similarity and difference in anti-plane surface waves propagation in an elastic half-space within the framework of of Gurtin-Murdoch surface elasticity and the lattice dynamics.

Statement of the problem

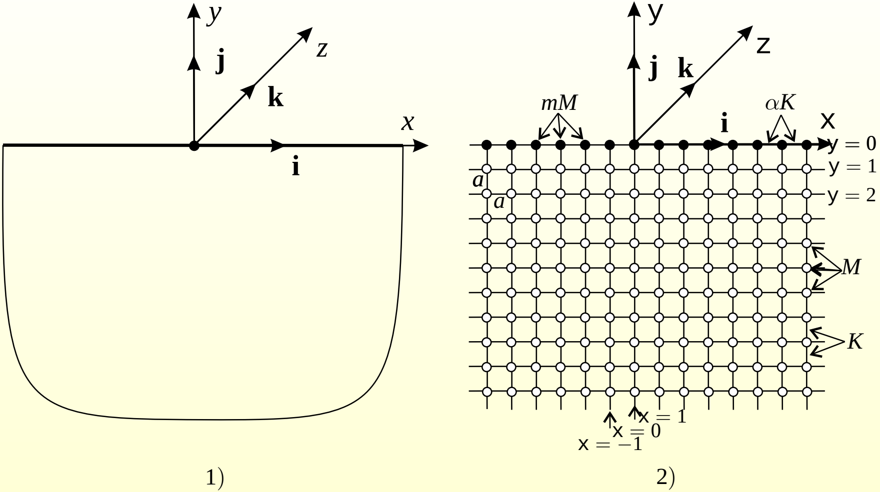

Figure: 1) Half-space with surface stresses and 2) a square lattice with different particles at the surface.

Few references

Surface elasticity

- M. E. Gurtin, A. I. Murdoch, A continuum theory of elastic material surfaces, *Arch. Ration. Mech. Analysis.* 57 (4) (1975) 291–323.
- M. E. Gurtin, A. I. Murdoch, Surface stress in solids, *Int. J. Solids Struct.* 14 (6) (1978) 431–440.

Lattice dynamics

- Born, M., Huang, K., 1985. *Dynamical Theory of Crystal Lattices*. The International Series of Monographs on Physics. Oxford Classic Texts in the Physical Sciences, The Clarendon Press, Oxford University Press, Oxford.
- Brillouin, L., 1946. *Wave Propagation in Periodic Structures: Electric Filters and Crystal Lattices*. McGrow-Hill, New York.

References on anti-plane surface waves

- F. Jia, Z. Zhang, H. Zhang, X.-Q. Feng, B. Gu, Shear horizontal wave dispersion in nanolayers with surface effects and determination of surface elastic constants, *Thin Solid Films* **645** (2018) 134 – 138.
- V. A. Eremeyev, G. Rosi, S. Naili, Surface/interfacial anti-plane waves in solids with surface energy, *Mech. Res. Comm.* **74** (2016) 8–13.
- V. A. Eremeyev, G. Rosi, S. Naili, Comparison of anti-plane surface waves in strain-gradient materials and materials with surface stresses. *Math. Mech. Solids* **24** (2019) 2526–2535
- Eremeyev, V.A., Sharma, B.L., Anti-plane surface waves in media with surface structure: Discrete vs. continuum model. *Int. J. Engng Science* **143** (2019) 33–38.

Gurtin-Murdoch model of the surface elasticity

We consider infinitesimal deformations of an elastic solid which are described by the displacement field

$$\mathbf{u} = \mathbf{u}(\mathbf{x}, t), \tag{1}$$

where $\mathbf{u}$ is twice differentiable vector-function of displacements, $\mathbf{x}$ is the position vector and t is time.
Within the Gurtin–Murdoch approach in the bulk, we have classic constitutive equations of an isotropic solid

$$\mathcal{W} = \mu \mathbf{e} : \mathbf{e} + \frac{1}{2}\lambda(\operatorname{tr}\mathbf{e})^2, \quad \boldsymbol{\sigma} \equiv \frac{\partial \mathcal{W}}{\partial \mathbf{e}} = 2\mu\mathbf{e} + \lambda\,\mathbf{I}\operatorname{tr}\mathbf{e}, \tag{2}$$

where $\mathcal{W}$ is the strain energy density, λ and μ are Lamé moduli, $\boldsymbol{\sigma}$ is the stress tensor, $\mathbf{e}$ is the strain tensor. The kinetic energy density is given by

$$\mathcal{K} = \frac{1}{2}\rho\dot{\mathbf{u}} \cdot \dot{\mathbf{u}}, \tag{3}$$

where ρ is the mass volume density.

Surface energies

Additionally, we introduce the surface strain energy density $\mathcal{W}_s$ and surface stress tensor $\mathbf{s}$ are defined as follows

$$\begin{aligned} \mathcal{W}_s &= \mu_s \boldsymbol{\epsilon} : \boldsymbol{\epsilon} + \frac{1}{2}\lambda_s (\operatorname{tr}\boldsymbol{\epsilon})^2, \\ \mathbf{s} &\equiv \frac{\partial \mathcal{W}_s}{\partial \boldsymbol{\epsilon}} = \mu_s \boldsymbol{\epsilon} + \lambda_s \mathbf{P}(\operatorname{tr}\boldsymbol{\epsilon}), \\ \boldsymbol{\epsilon} &= \frac{1}{2}\left(\mathbf{P}\cdot(\nabla_s \mathbf{u}) + (\nabla_s \mathbf{u})^T \cdot \mathbf{P}\right), \end{aligned} \tag{4}$$

where λ_s and μ_s are the surface elastic moduli, tr is the trace operator, ∇_s is the surface nabla operator, $\mathbf{P} \equiv \mathbf{I} - \mathbf{n} \otimes \mathbf{n}$, $\mathbf{n}$ is the unit vector of outer normal to ∂V. In addition, we take into account the surface mass density and introduce the following formula for surface kinetic energy density

$$\mathcal{K}_s = \frac{1}{2} m \dot{\mathbf{u}} \cdot \dot{\mathbf{u}}\Big|_{\mathbf{x}\in\partial V}, \tag{5}$$

where m is the surface mass density and ∂V is the boundary of V.

Variational statement

Motion and natural boundary equations can be derived using the least action principle with the functional

$$\mathcal{L} = \int_0^T \int_V (\mathcal{K} - \mathcal{W})\, dV\, dt + \int_0^T \int_{\partial V} (\mathcal{K}_s - \mathcal{W}_s)\, da\, dt. \qquad (6)$$

Anti-plane surface waves in an elastic half-space

Let us consider stationary waves of an elastic half-space $x_1 \leq 0$. In what follows we use the Cartesian coordinates x_1, x_2 and x_3 with the basis $\mathbf{i}_k$, $k = 1, 2, 3$.
For the anti-plane motion, the vector of displacement takes the form

$$\mathbf{u} = u(x_1, x_2, t)\mathbf{i}_3. \tag{7}$$

From (7), it follows that

$$\nabla\mathbf{u} = u_{,\alpha}\mathbf{i}_3 \otimes \mathbf{i}_\alpha = \mathbf{i}_3 \otimes \nabla u, \quad \nabla \cdot \mathbf{u} = 0,$$

$$\mathbf{e} = \frac{1}{2}(\nabla u \otimes \mathbf{i}_3 + \mathbf{i}_3 \otimes \nabla u), \quad \nabla\mathbf{e} = \frac{1}{2}(\mathbf{i}_3 \otimes \nabla\nabla u + \nabla u_{,\alpha}\mathbf{i}_3 \otimes \mathbf{i}_\alpha)$$

Hereafter, we used the notation $u_{,\alpha} = \frac{\partial u}{\partial x_\alpha}$, and Greek indices take values 1, or 2. $\nabla \cdot \mathbf{u}$ is the divergence of $\mathbf{u}$.
Under assumption that a steady state has been reached, we may search displacement of the form

$$u = U(x_1) \exp\left[i(kx_2 - \omega t)\right], \tag{8}$$

where k is the wavenumber, ω is the circular velocity, and $i = \sqrt{-1}$.

Surface elasticity

For the anti-plane shear deformation (7), the motion equations and the boundary conditions reduce to

$$\rho\ddot{u} = \mu\Delta u, \tag{9}$$

$$-m\ddot{u} + \mu_s u_{,22} = \mu u_{,1}. \tag{10}$$

Substituting (8) into (9), we obtain the ordinary differential equation with respect to U

$$\left[\mu(\partial^2 - k^2) + \rho\omega^2\right] U = 0. \tag{11}$$

Assuming that the displacement decays exponentially with distance from the half-space surface, we find the solution of (11)

$$U = U_0 \exp\left[\sqrt{k^2 - \omega^2/c_T^2}\, x_1\right],$$

where U_0 is an amplitude and $c_T = \sqrt{\frac{\mu}{\rho}}$ is the phase velocity of shear waves in the bulk.

Solution

As a result, we obtain the expression for an anti-plane surface wave of the form

$$u = U_0 \exp\left[\sqrt{k^2 - \omega^2/c_T^2}\,x_1\right] \exp\left[i(kx_2 - \omega t)\right]. \tag{12}$$

Substituting (12) into (10), we obtain the dispersion equation

$$D_S(\omega, k) \equiv m\omega^2 - \mu_s k^2 - \mu\sqrt{k^2 - \frac{\omega^2}{c_T^2}} = 0. \tag{13}$$

Dispersion relation

The latter equation transforms to

$$c^2 = \frac{\mu_s}{m} + \frac{\mu}{m}\frac{1}{|k|}\sqrt{1 - \frac{c^2}{c_T^2}} \tag{14}$$

with solution of the form

$$|k| = \frac{\mu\sqrt{1 - \frac{c^2}{c_T{}^2}}}{m(c^2 - c_S^2)}, \tag{15}$$

where $c_S = \sqrt{\mu_s/m}$ is the shear wave velocity in the thin film associated with the Gurtin–Murdoch model. Obviously, the wavenumber k is real if and only if

$$c \leq c_T, \quad c > c_S. \tag{16}$$

Square lattice

The positions of the lattice particles are described through its lattice coordinates $\mathsf{x} \in \mathbb{Z}$, $\mathsf{y} \leq 0$, $\mathsf{y} \in \mathbb{Z}$. The lattice mostly consists of identical particles of mass M connected to each other by linearly elastic bonds (springs) of stiffness K. In order to model surface tension we assume that the free surface $\mathsf{y} = 0$ is constituted by particles with masses mM and bonds with spring constant αK, whereas m and α are dimensionless parameters. The anti-plane displacement of a particle, indexed by its lattice coordinates $\mathsf{x} \in \mathbb{Z}$, $\mathsf{y} \in \mathbb{Z}$, is denoted by $\mathsf{u}_{\mathsf{x},\mathsf{y}}$. Herein and after, let $\mathbb{Z}$ denote the set of integers. The motion equation for square lattice is given by

$$M\ddot{\mathsf{u}}_{\mathsf{x},\mathsf{y}} = K\left(\mathsf{u}_{\mathsf{x}+1,\mathsf{y}} + \mathsf{u}_{\mathsf{x}-1,\mathsf{y}} + \mathsf{u}_{\mathsf{x},\mathsf{y}+1} + \mathsf{u}_{\mathsf{x},\mathsf{y}-1} - 4\mathsf{u}_{\mathsf{x},\mathsf{y}}\right) \qquad (17)$$

for $\mathsf{x} \in \mathbb{Z}$, $\mathsf{y} < 0$, $\mathsf{y} \in \mathbb{Z}$. On the free surface that is for $\mathsf{x} \in \mathbb{Z}$, $\mathsf{y} = 0$ we have

$$mM\ddot{\mathsf{u}}_{\mathsf{x},\mathsf{y}} = \alpha K\left(\mathsf{u}_{\mathsf{x}+1,\mathsf{y}} + \mathsf{u}_{\mathsf{x}-1,\mathsf{y}} - 2\mathsf{u}_{\mathsf{x},\mathsf{y}}\right) + K\left(\mathsf{u}_{\mathsf{x},\mathsf{y}-1} - \mathsf{u}_{\mathsf{x},\mathsf{y}}\right). \qquad (18)$$

Surface wave

Let us consider the discrete analogue of the surface wave form, i.e.,

$$\mathsf{u}_{\mathsf{x},\mathsf{y}} = \mathsf{u}_0 \exp(i\xi \mathsf{x} - i\omega t) \exp(\eta \mathsf{y}), \tag{19}$$

where ξ is the discrete wave number, $\xi \in (-\pi, \pi)$, and η is assumed to be positive.
It is found that ω and η satisfy the two equations

$$-M\omega^2 = K\left(2\cos\xi + 2\cosh\eta - 4\right), \tag{20}$$

$$-mM\omega^2 = \alpha K\left(2\cos\xi - 2\right) + K(\exp(-\eta) - 1). \tag{21}$$

Dispersion relation

Motivated by a continuum context, let

$$M = \rho a^3, \quad K = \mu a, \tag{22}$$

where ρ and μ are the mass density and shear modulus introduced in previous Section. Then from (35) and (36) we get

$$\omega^2 = \frac{c_T^2}{a^2}\left(4 - 2\cos\xi - 2\cosh\eta\right), \tag{23}$$

$$\omega^2 = 2\frac{\alpha c_T^2}{ma^2}\left(1 - \cos\xi\right) + \frac{c_T^2}{ma^2}(1 - \exp(-\eta)). \tag{24}$$

These two equations result in a dispersion relation for the surface waves on square lattice half-plane with surface structure. As ξ and η play a role of k and γ, respectively, Eqs. (23) and (24) are the discrete analogues of the dispersion relation for the elastic half-space with surface stresses.

Dispersion curves

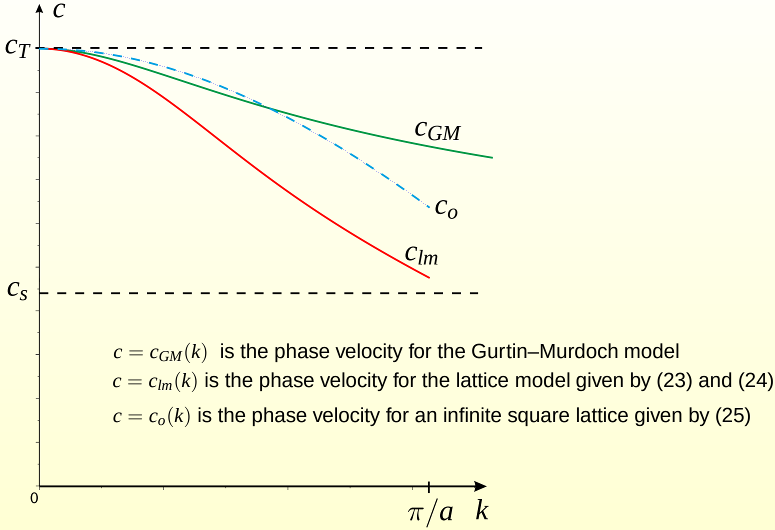

Figure: Phase velocity vs. wave number for discrete and continuum model.

Dispersion curves: parameters

In order to compare the dispersion relation (15) with (23) and (24) we substitute $\xi = ka$ and consider k in the range $k \in [0, \pi/a]$. The dashed blue curve in Fig. 2 corresponds to the equation

$$c = c_o(k) \equiv 2c_T \frac{\left|\sin\left(\frac{ka}{2}\right)\right|}{ka}, \qquad (25)$$

which gives the phase velocity c_o for an infinite square lattice. Here we used the following values of material parameters: $c_T = 1$, $c_s = \sqrt{0.2}$, $r = 0.005$ for continuum model and $a = 0.01$, $\alpha = 0.1$ and $m = 0.5$ for the lattice. Note that these parameters satisfy the relation

$$c_{GM}(0) = c_T = c_{lm}(0). \qquad (26)$$

From (26) we get the relation

$$c_T = \sqrt{\frac{\mu}{\rho}} = a\sqrt{\frac{K}{M}},$$

which is consistent with assumption (22). So for long wave approximation ($k \approx 0$) we have good coincidence between models.

Scaling law

Clearly, while keeping m and α constant as $a \to 0$ we cannot obtain anti-plane surface wave as a continuum limit of the discrete model, since in this case we recover an elastic half-space for which it is well known that such waves *do not exist*. Hence, to capture the behaviour of the Gurtin–Murdoch model one needs to apply an appropriate scaling for m and α.

Here we propose the following scaling law

$$\alpha = \frac{1}{a}\frac{\mu_s}{\mu}, \quad m = \frac{1}{a}\frac{\rho_s}{\rho}. \tag{27}$$

With (27) we get that the surface bond stiffness became constant at $a \to 0$, $\alpha K = \mu_s$, whereas the mass of surface particles $mM = \rho_s a^2$. As a results, for c_s we have

$$c_s = \sqrt{\frac{\mu_s}{\rho_s}} = \sqrt{\frac{\alpha K}{mM}}\, a = \sqrt{\frac{\alpha}{m}}\, c_T. \tag{28}$$

So the scaling law (27) gives the second correspondence between continuum and discrete model.

Dispersion curves

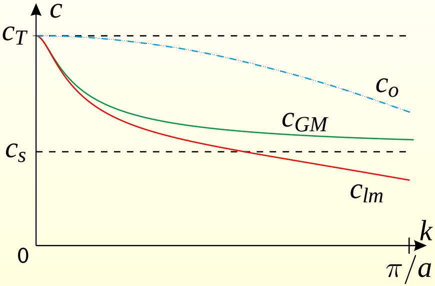

Figure: Phase velocity vs. wave number for discrete and continuum model for $a = 0.001$ (on the left) and $a = 0.0001$ (on the right).

Comparison with Toupin–Mindlin model

Let us note that the relations between the linear Gurtin–Murdoch model and the lattice model in a certain sense similar to relations between surface elasticity and the Toupin–Mindlin linear strain gradient elasticity. Indeed, both theories possess surface energy and the corresponding dispersion relations for anti-plane surface waves are qualitatively similar for both models. The relations between material parameters of these models can be obtained from the equations

$$c_{GM}(0) = c_T = c_{TM}(0), \quad \lim_{k\to\infty} c_{GM}(k) = c_s = \lim_{k\to\infty} c_{TM}(k),$$

where $c_{TM} = c_{TM}(k)$ is the phase velocity for the Toupin–Mindlin constitutive relations. Nevertheless, there is difference in decay with the depth, so their correspondence is not straightforward as in presented case here. In addition, for the discrete model $c_{lm}(k)$ is defined for the finite range of k.

Surface interface

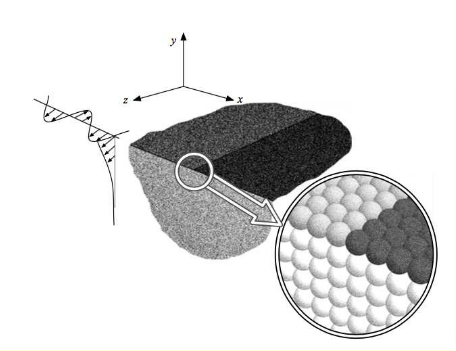

Figure: Geometry of the three dimensional lattice half space is shown schematically by placing a cutting section along x-y plane. On the right side (by zooming into the central portion), an atomic/particle based discrete model of an elastic half space with surface interface is shown. The kinematics assumed is that if anti-plane motion, i.e. the displacement occurs along z direction only, as shown on the left, while it is independent of the z coordinate.

Surface interface

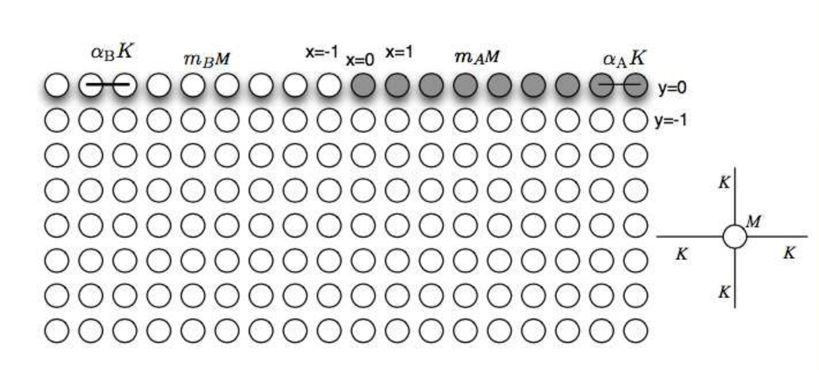

Figure: An illustration of the geometry of the lattice half space with structured surface interface on free boundary. A two dimensional projection is schematically illustrated from previous figure.

Equation of motion

The motion equation for square lattice is given by

$$M\ddot{u}_{x,y} = K\left(u_{x+1,y} + u_{x-1,y} + u_{x,y+1} + u_{x,y-1} - 4u_{x,y}\right) \tag{29}$$

for $x \in \mathbb{Z}^+$, $y < 0$, $y \in \mathbb{Z}$. On the free surface that is for $0 < x \in \mathbb{Z}$, $y = 0$ we have

$$m_A M\ddot{u}_{x,y} = \alpha_A K\left(u_{x+1,y} + u_{x-1,y} - 2u_{x,y}\right) + K\left(u_{x,y-1} - u_{x,y}\right), \tag{30}$$

for $x \in \mathbb{Z}^-$, $y = 0$ we have

$$m_B M\ddot{u}_{x,y} = \alpha_B K\left(u_{x+1,y} + u_{x-1,y} - 2u_{x,y}\right) + K\left(u_{x,y-1} - u_{x,y}\right). \tag{31}$$

for $x = 0$, $y = 0$ we have

$$m_A M\ddot{u}_{x,y} = \alpha_A K\left(u_{x+1,y} + u_{x-1,y} - 2u_{x,y}\right) + K\left(u_{x,y-1} - u_{x,y}\right). \tag{32}$$

Incident surface wave

Let us consider the incident surface wave

$$\mathsf{u}^{\mathsf{in}}_{\mathsf{x,y}} = \mathrm{A}\exp(-i\xi_{\mathsf{in}}\mathsf{x} - i\omega t)\exp(\eta_{\mathsf{in}}\mathsf{y}), \tag{33}$$

where ξ_{in} is the discrete wave number from the right side such that $\mathsf{v}_g(\xi_{\mathsf{in}}) < 0$, $\xi_{\mathsf{in}} \in (0, \pi)$, and η_{in} is assumed to be positive. Let

$$\mathrm{\omega} = \omega a/c. \tag{34}$$

It is found that $\mathrm{\omega} = \mathrm{\omega}_A(\xi_{\mathsf{in}})$ and $\eta_{\mathsf{in}} = \eta_A(\xi_{\mathsf{in}})$ satisfy the two equations

$$-\mathrm{\omega}^2 = (2\cos\xi_{\mathsf{in}} + 2\cosh\eta_{\mathsf{in}} - 4)\,, \tag{35}$$

$$-m_A\mathrm{\omega}^2 = \alpha_A\,(2\cos\xi_{\mathsf{in}} - 2) + (\exp(-\eta_{\mathsf{in}}) - 1). \tag{36}$$

Lattice strip with the interface

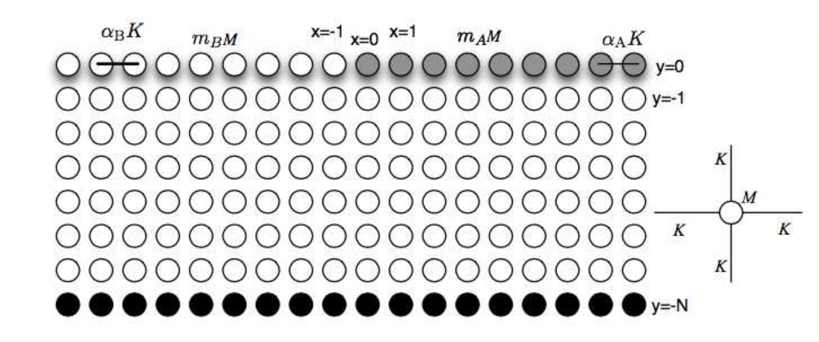

Figure: An illustration of the geometry of the lattice strip with structured surface interface on free boundary.

Reflectance, transmittance, leaked energy flux

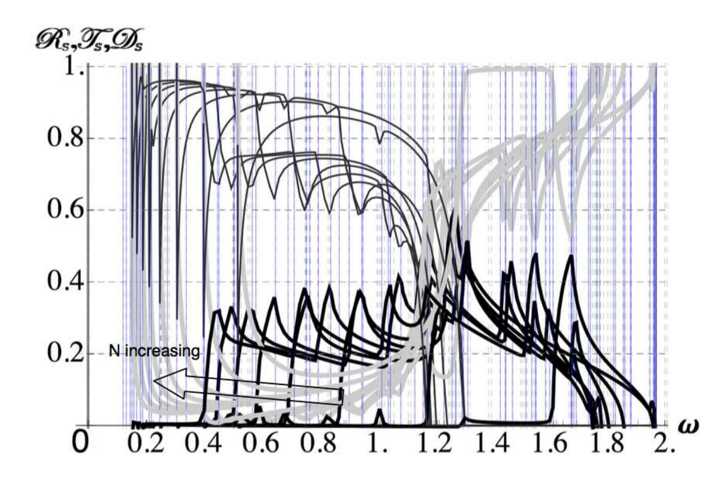

Figure: The reflectance (black thin curves), transmittance (gray thick curves), and the leaked energy flux (black thick curves) by superposition of the eight values of N; $\mathsf{N} = 2, 3, \ldots, 8$ with $\alpha_A = 1.4$, $\alpha_B = 1.5$, $m_A = 2$, $m_A = 5$.

Future Steps

- Surface interface — reflection and transmission of surface waves across the surface interface using both discrete and continuum model;
- "Full" description of surface waves within both theories;
- Complex lattices;
- Complex particle interactions.

References:

- Eremeyev, V.A., Sharma, B.L., Anti-plane surface waves in media with surface structure: Discrete vs. continuum model. *Int. J. Engng Science* **143** (2019) 33–38.
- Sharma, B.L., Eremeyev, V.A., Wave transmission across surface interfaces in lattice structures. *Int. J. Engng Science* **145** (2019) 103173.

Conclusions

- For anti-plane surface waves, we demonstrate the essential similarity between dispersion relations derived within both discrete and continuum model of a surface structure. We consider a square semi-infinite lattice with a surface row of particles which properties are different from ones in the bulk, and the linear Gurtin–Murdoch model of surface elasticity. These different models can capture material behavior related to presence of surface energy.
- On the other hand the transition from the lattice model to the Gurtin–Murdoch model is not straightforward, as it requires additional assumptions on the dependence of surface particles' mass and surface bond stiffness on the lattice cell length a.

Thank you for your attention!

Further Questions:

eremeyev.victor@gmail.com