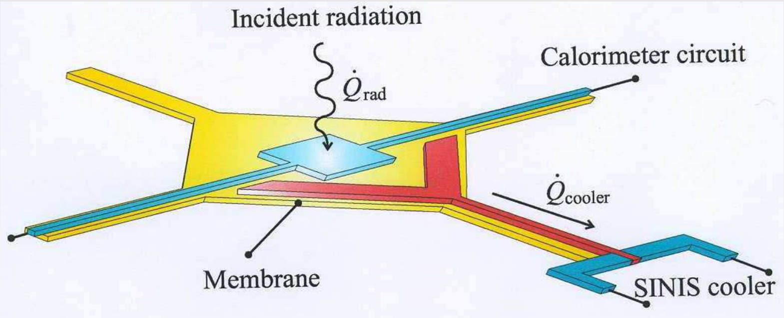
Dynamic defects and heat transport in nanoscopic amorphous membranes

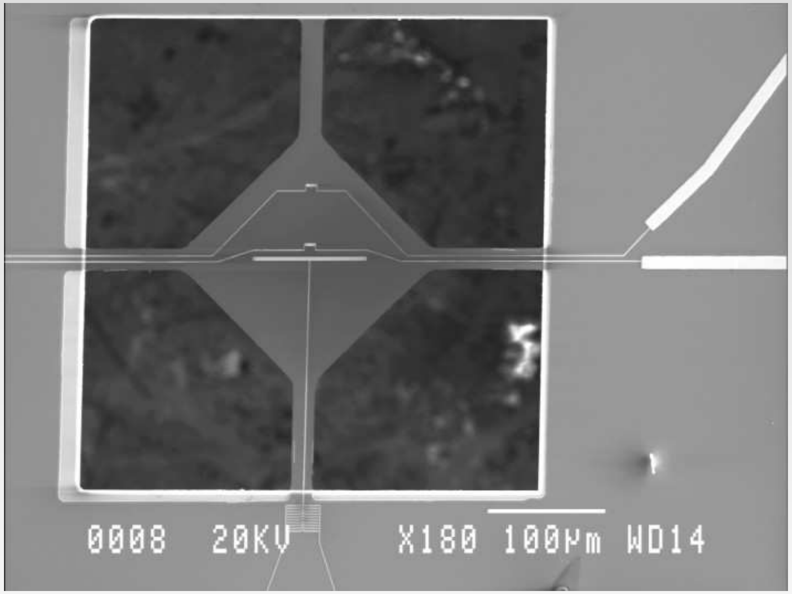
Dragoş-Victor Anghel

Department of Theoretical Physics, National Institute of Physics and Nuclear Engineering–“Horia Hulubei”, Bucharest, Romania

Starting point

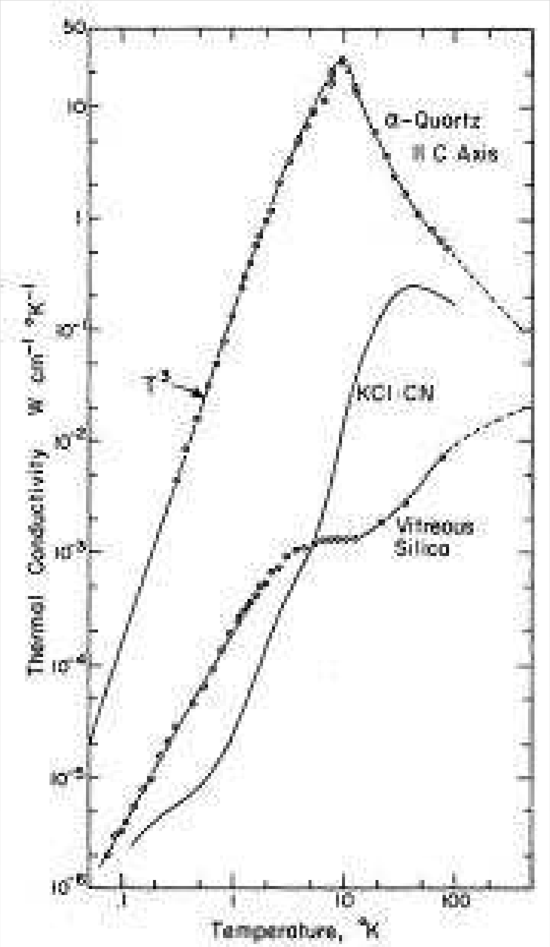
Calculation of the thermal properties and noise in nano-detectors

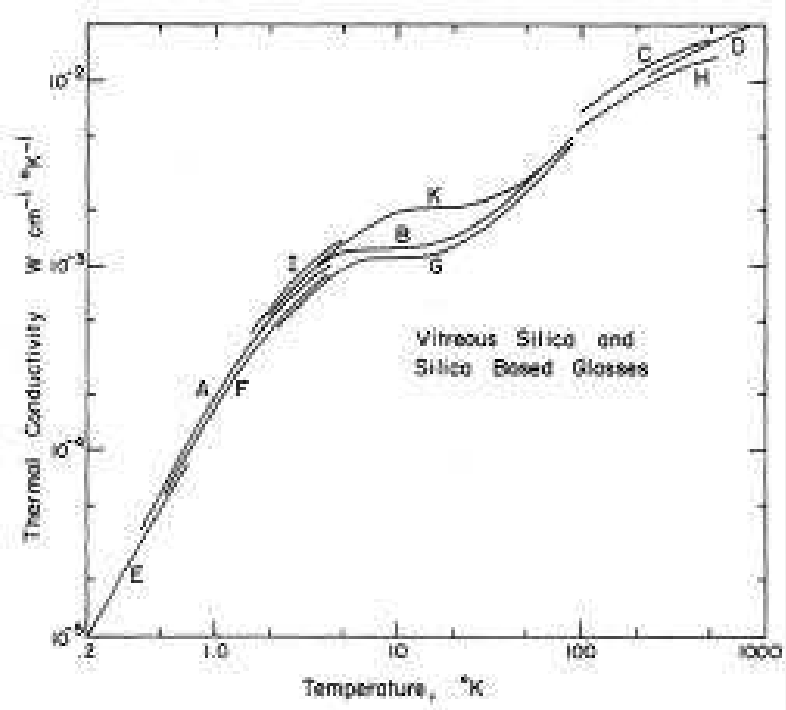




Pictures courtuasy to M. Leivo, A. Luukanen and J. P. Pekola

Amorphous materials

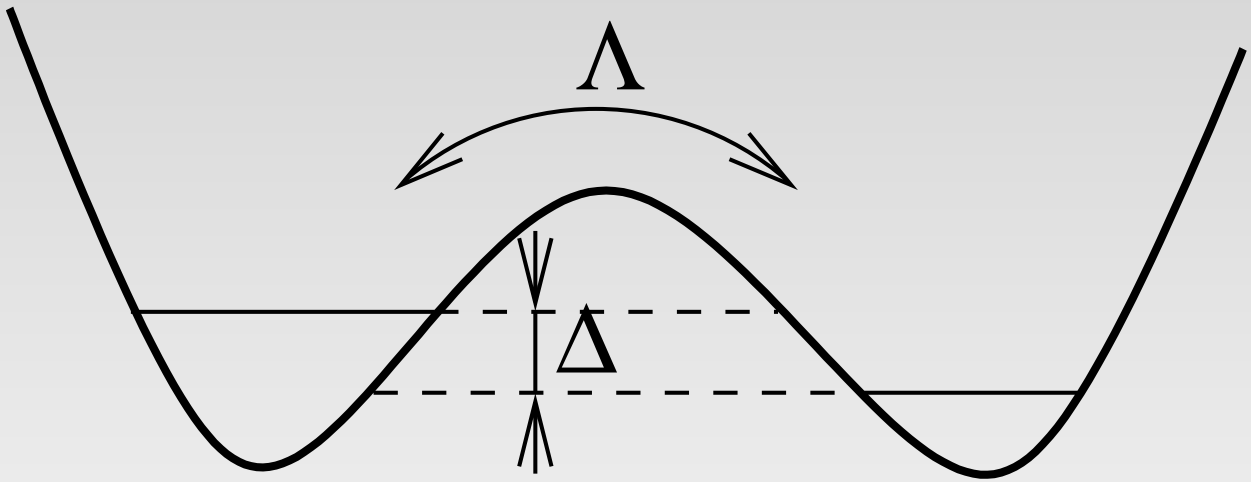




Zeller & Pohl, Phys. Rev. B **4**, 2029 (1971).

The dynamic defects

It is assumed that the solid contains an ensemble of two-level systems (TLS).



The two-well potential of the TLS

Properties of the TLSs

Hamiltonian : $$H_{\text{TLS}} = \frac{\Delta}{2}\sigma_z - \frac{\Lambda}{2}\sigma_x \equiv \frac{1}{2}\begin{pmatrix} \Delta & -\Lambda \\ -\Lambda & -\Delta \end{pmatrix}$$

$$p = \Lambda/\Delta$$

Eigenvectors : $$|\downarrow\rangle = \frac{\sqrt{\sqrt{1+p^2}+1}}{\sqrt{2}(1+p^2)^{1/4}} \cdot \begin{pmatrix} \frac{p}{1+\sqrt{1+p^2}} \\ 1 \end{pmatrix}$$

$$|\uparrow\rangle = \frac{\sqrt{\sqrt{1+p^2}-1}}{\sqrt{2}(1+p^2)^{1/4}} \cdot \begin{pmatrix} \frac{p}{1-\sqrt{1+p^2}} \\ 1 \end{pmatrix}$$

Eigenvalues and probability distribution of TLSs

Diagonalization:

$$H'_{\rm TLS} = O^T H_{\rm TLS} O = \frac{\epsilon}{2}\sigma_z = \frac{1}{2}\left(\begin{array}{cc} \epsilon & 0 \\ 0 & -\epsilon \end{array}\right)$$

Probability distribution:

$$P(\Delta, \Lambda) = P_0/\Lambda, \qquad P(\epsilon, u) = \frac{P_0}{u\sqrt{1-u^2}}$$

Notations:

$$\epsilon = \sqrt{\Delta^2 + \Lambda^2}, \qquad u = \frac{\Delta}{\epsilon}$$

Phonon-TLS interaction

$$\text{Interaction :} \qquad H_1 = \frac{\delta}{2}\sigma_z \equiv \frac{1}{2}\begin{pmatrix} \delta & 0 \\ 0 & -\delta \end{pmatrix}$$

$$H_1' \equiv O^T H_1 O = \frac{\delta}{2\epsilon}\begin{pmatrix} \Delta & -\Lambda \\ -\Lambda & -\Delta \end{pmatrix}$$

$$\delta = 2\gamma_{ij}S_{ij}, \qquad S_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$$

TLS-phonon interaction in bulk:

$$\delta_\sigma = 2N_\sigma\gamma_\sigma k_\sigma,\ \sigma = t, l,\ N_\sigma = \text{phonon normalization}$$

Transition rates and physical results

$$\langle n_{\mathbf{k}\sigma}+1,\downarrow|H_1'|n_{\mathbf{k}\sigma}\uparrow\rangle = -\sqrt{\frac{\hbar k}{2V\rho c_\sigma}}\gamma_\sigma\frac{\Lambda}{\epsilon}\sqrt{n_{\mathbf{k}\sigma}+1}$$

$$\Gamma_{\rm em}(\epsilon,\mathbf{k},\sigma) = \gamma_\sigma^2\frac{\pi k}{V\rho c_\sigma}\frac{\Lambda^2}{\epsilon^2}(n_{\mathbf{k}\sigma}+1)\delta(\hbar c_\sigma k-\epsilon)$$

$$\Gamma_{\rm abs}(\epsilon,\mathbf{k},\sigma) = \gamma_\sigma^2\frac{\pi k}{V\rho c_\sigma}\frac{\Lambda^2}{\epsilon^2}n_{\mathbf{k}\sigma}\delta(\hbar c_\sigma k-\epsilon)$$

$$\tau_\epsilon^{-1} = \left(\frac{\gamma_l^2}{c_l^5}+\frac{2\gamma_t^2}{c_t^5}\right)\frac{\Lambda^2\epsilon}{2\pi\rho\hbar^4}\cdot\coth\left(\frac{\beta\epsilon}{2}\right)$$

$$\tau_{\mathbf{k}\sigma}^{-1} = \frac{\pi\hbar\omega_{k,\sigma}}{\hbar\rho c_\sigma^2}\cdot\gamma_\sigma^2 P_0\cdot\tanh\left(\frac{\beta\hbar\omega_{k,\sigma}}{2}\right)$$

$$\frac{\Delta c_\sigma}{c_\sigma} = \frac{\gamma_\sigma^2 P_0}{\rho c_\sigma^2}\ln\left(\frac{T}{T_0}\right)$$

$$\kappa(T) = \frac{\rho k_{\rm B}{}^3}{6\pi\hbar^2}\left(\frac{c_l}{\gamma_l^2 P_0}+\frac{2c_t}{\gamma_t^2 P_0}\right)$$

General phonon-TLS interaction

In general,

$$\delta = 2\gamma_{ij}S_{ij} \equiv 2[\gamma] : [S]$$

$[S]$ is a symmetric tensor
$\Downarrow$
$[\gamma]$ is a symmetric *tensor*, so that
δ is a *scalar*
$[\gamma]$ characterises the TLS, so we have to build its components from *general physical characteristics of the TLS*.

Phonon-TLS interaction tensor

We associate a direction $\hat{\mathbf{t}}$ to the TLS:

$$\hat{\mathbf{t}} \equiv \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix}$$

and we build the simplest symmetric tensor,

$$[T] = \begin{pmatrix} t_x^2 & t_x t_y & t_x t_z \\ t_x t_y & t_y^2 & t_y t_z \\ t_x t_z & t_y t_z & t_x^2 \end{pmatrix} \equiv \hat{\mathbf{t}} \cdot \hat{\mathbf{t}}^T,$$

Abbreviated subscript notations

We switch to abbreviated subscript notations and write

$$\mathbf{S} \equiv (S_{xx}, S_{yy}, S_{zz}, 2S_{yz}, 2S_{zx}, 2S_{xy})^T$$
$$\mathbf{T} \equiv (T_{xx}, T_{yy}, T_{zz}, 2T_{yz}, 2T_{zx}, 2T_{xy})^T$$

A general interaction tensor would have the form

$$\gamma \equiv [R]^T \cdot \mathbf{T}$$

So, finally,

$$\delta = 2\mathbf{T}^T \cdot [R] \cdot \mathbf{S}.$$

Properties of γ

$$\delta = 2\mathbf{T}^T \cdot [R] \cdot \mathbf{S}$$ is a scalar,

so the properties of $[R]$ can be determined from the invariance of δ to a variety of coordinates transformations.

$$\mathbf{S}' \equiv [N]\mathbf{S},\ \mathbf{T}' = [N]\mathbf{T} \qquad \Rightarrow \qquad [N]^T \cdot [R] \cdot [N] = [R]\,.$$

Similar to the tensor of elastic constants, where

$$u = \frac{1}{2}\mathbf{S}^T[c]\mathbf{S} \ \Rightarrow\ [N]^T \cdot [c] \cdot [N] = [c]$$

Interaction in an isotropic medium

If the medium is isotropic, then

$$[R] = \begin{pmatrix} \zeta' + 2\xi' & \zeta' & \zeta' & 0 & 0 & 0 \\ \zeta' & \zeta' + 2\xi' & \zeta' & 0 & 0 & 0 \\ \zeta' & \zeta' & \zeta' + 2\xi' & 0 & 0 & 0 \\ 0 & 0 & 0 & \xi' & 0 & 0 \\ 0 & 0 & 0 & 0 & \xi' & 0 \\ 0 & 0 & 0 & 0 & 0 & \xi' \end{pmatrix} \equiv \tilde{\gamma} \cdot [r]$$

where we defined with $\tilde{\gamma} \equiv \zeta' + 2\xi'$ and we shall use the notations $\zeta \equiv \zeta'/\tilde{\gamma}$ and $\xi \equiv \xi'/\tilde{\gamma}$.

Interaction Hamiltonian

Introducing the excitation and de-excitation operators for the TLS,

$$a^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \; a = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

we write the interaction hamiltonian in the second quantization as

$$\begin{aligned} \tilde{H}_1 &= \frac{\tilde{\gamma}\Delta}{\epsilon}\mathbf{T}^T \cdot [r] \cdot \sum_\mu \left[\mathbf{S}_\mu b_\mu + \mathbf{S}^\star_\mu b^\dagger_\mu\right](2a^\dagger a - 1) \\ &\quad -\frac{\tilde{\gamma}\Lambda}{\epsilon}\mathbf{T}^T \cdot [r] \cdot \sum_\mu \left[\mathbf{S}_\mu b_\mu + \mathbf{S}^\star_\mu b^\dagger_\mu\right](a^\dagger + a) \end{aligned}$$

Results:

$$\langle n_{\mathbf{k}\sigma}, \uparrow | \tilde{H}_1 | n_{\mathbf{k}\sigma}+1, \downarrow\rangle = -\frac{\tilde{\gamma}\Lambda}{\epsilon}\sqrt{\frac{\hbar n_{\mathbf{k}\sigma}}{2V\rho\omega_{\mathbf{k}\sigma}}}\mathbf{T}^T \cdot [r] \cdot \mathbf{S}_{\mathbf{k}\sigma}$$

We take the modulus square and average over $\hat{\mathbf{t}}$ to get:

$$\overline{\Gamma}_{|n_{\mathbf{k}\sigma},\uparrow\rangle,|n_{\mathbf{k}\sigma}+1,\downarrow\rangle} = C_\sigma\tilde{\gamma}^2\frac{n_{\mathbf{k}\sigma}\pi k}{\rho c_\sigma} \cdot \frac{\Lambda^2}{\epsilon^2}\delta(\hbar\omega_{\mathbf{k}\sigma} - \epsilon)$$

$$\overline{\Gamma}_{|n_{\mathbf{k}\sigma}+1,\uparrow\rangle,|n_{\mathbf{k}\sigma},\downarrow\rangle} = C_\sigma\tilde{\gamma}^2\frac{(n_{\mathbf{k}\sigma}+1)\pi k}{V\rho c_\sigma} \cdot \frac{\Lambda^2}{\epsilon^2}\delta(\hbar\omega_{\mathbf{k}\sigma} - \epsilon)$$

with $C_l\tilde{\gamma}^2 = \gamma_l$ and $C_t\tilde{\gamma}^2 = \gamma_t$ where

$$C_l = \frac{2}{30}(15 - 40\xi + 32\xi^2), \; C_t = \frac{8}{30}\xi^2$$

Note: $C_l/C_t \geq 4/3$ for any ξ, *in agreement with experiment*.

Calculation of the parameters

From experiment (J. L. Black, Phys. Rev. B, **17**, 2704, 1978):

1. $P_0\gamma_l^2 = 1.4 \times 10^{-5}\ J/m^3, P_0\gamma_t^2 = 0.63 \times 10^{-5}\ J/m^3,$
2. $P_0\gamma_l^2 = 2.0 \times 10^{-5}\ J/m^3,\ P_0\gamma_t^2 = 0.89 \times 10^{-5}\ J/m^3$

$$\Downarrow$$

Both sets, almost the same solutions:

$$\xi_1 \approx 1.2, \qquad \zeta_1 \approx -1.4$$
$$\xi_2 \approx 0.55, \qquad \zeta_2 \approx -0.1$$

Scattering of waves

A longitudinal wave propagating along the x direction:

$$\mathbf{S} = (S,0,0,0,0,0)^T$$
$$\gamma = 2\tilde{\gamma}[t_x^2 + \zeta(t_y^2 + t_z^2)]S$$

is scattered by *any* TLS.

A transversal wave of $\mathbf{S} = (0,0,0,S,0,0)^T$

$$\gamma = 4\tilde{\gamma}t_y t_z S$$

is *not* scattered by TLSs perpendicular to the propagation direction or to the polarization direction.

Polarization of the TLS ensemble

If we apply a longitudinal strain along the x direction, $\mathbf{S} = (S, 0, 0, 0, 0, 0)^T$, this will change the asymetry of the TLS potential by

$$\gamma = 2\tilde{\gamma}[t_x^2 + \zeta(t_y^2 + t_z^2)]S,$$

So the change of Δ, and therefore of ϵ, of the TLS oriented along the strain direction might have an opposite sign as compared to the quantities corresponding to the TLSs perpendicular to the strain direction.

TLS-phonon interaction in membranes

$$\langle n_{\mathbf{k}\sigma},\uparrow|\tilde{H}_1|n_{\mathbf{k}\sigma}+1,\downarrow\rangle = -\frac{\tilde{\gamma}\Lambda}{\epsilon}\sqrt{\frac{\hbar n_{\mathbf{k}\sigma}}{2\rho\omega_{\mathbf{k}\sigma}}}\mathbf{T}^T\cdot[r]\cdot\mathbf{S}_{\mathbf{k}\sigma}$$

Notation: $M_\mu(\hat{\mathbf{t}}) = \mathbf{T}^T\cdot[r]\cdot\mathbf{S}_\mu$.

$$\tau_\epsilon^{-1} = \frac{\pi}{\rho}\frac{\tilde{\gamma}^2\Lambda^2}{\epsilon^2}\coth(\beta\epsilon/2)\sum_\mu\frac{1}{\omega_\mu}\langle|M_\mu|^2\rangle\delta(\hbar\omega_\mu-\epsilon)$$

$$\tau_\mu^{-1} = \frac{\pi\tilde{\gamma}^2VP_0}{\rho\omega_\mu}\langle|M_\mu|^2\rangle\tanh(\beta\hbar\omega/2)$$

$$\kappa = \frac{\hbar^2\rho}{16\pi^2\tilde{\gamma}^2VP_0}\frac{1}{k_\mathrm{B}T^2}\sum_{n,\sigma}\int_0^\infty dk_{\|}\left(\frac{\partial\omega_\mu}{\partial k_{\|}}\right)^2\frac{k_{\|}\omega_\mu^3}{\langle|M_\mu|^2\rangle}\frac{\coth(\beta\hbar\omega/2)}{\sinh^2(\beta\hbar\omega/2)}$$

Low temperature expansions

Horisontal shear (h) mode:

$$\tau_{h,0,k_{\|}} = \frac{\hbar\rho c_t^2}{\pi\tilde{\gamma}^2 P_0} \frac{1}{C_t} \frac{\coth(\beta\hbar\omega/2)}{\hbar\omega}$$

Symmetric (s) mode:

$$\tau_{s,0,k_{\|}} = \frac{\hbar\rho c_t^2}{\pi\tilde{\gamma}^2 P_0} \frac{1}{C_s} \frac{\coth(\beta\hbar\omega/2)}{\hbar\omega}$$

Antisymmetric (a) mode:

$$\tau_{a,0,k_{\|}} = \frac{\hbar\rho c_t^2}{\pi\tilde{\gamma}^2 P_0} \frac{1}{C_a} \frac{\coth(\beta\hbar\omega/2)}{\hbar\omega}$$

$$\kappa \approx \frac{k_B^2 \rho c_t^2}{4\pi^2\hbar\tilde{\gamma}^2 P_0} T \sum_\sigma \frac{3 - 2\ln(x_{\sigma,0,k_{c,h}})}{C_\sigma}, \; x_{\sigma,0,k_{c,\sigma}} \equiv \beta\hbar\omega_{\sigma,0,k_{c,\sigma}} \ll 1$$

Conclusions

- We introduced a model of interaction of a TLS with general strain fields.

- For this we associated to the TLS a direction in space, $\hat{\mathbf{t}}$, and a matrix of coupling constants, $[R]$ (in abbreviated subscript notations).

- The matrix of coupling constants has the same properties as, for example, the matrix of elastic stiffness constant, $[c]$.

- The TLS-phonon interaction in bulk is re-obtained from our model as an average interaction over the directions of the TLS.

- We calculated the thermal properties of amorphous, nanoscopic membranes.

- Anisotropy of TLS-sound wave interaction appears naturally.
- We predict the polarization of the TLS ensemble in a strained body.

Resources

1. D. V. Anghel, T. Kühn, Y. M Galperin, and M. Manninen, *The tensor of interaction of a two-level system with an arbitrary strain field*, J. Phys.: Conf. Series **92**, 12133 (2007); arXiv:0710.0720.

2. T. Kühn, D. V. Anghel, Y. M Galperin, and M. Manninen, *Interaction of Lamb modes with two-level systems in amorphous nanoscopic membranes*, Phys. Rev. B **76**, 165425 (2007); arXiv:0705.1936.

3. D. V. Anghel and T. Kühn, *Quantization of the elastic modes in an isotropic plate*, J. Phys. A: Math. Theor. **40**, 10429 (2007); cond-mat/0611528.

4. D. V. Anghel, T. Kühn, Y. M Galperin, and M. Manninen, *Interaction of two-level systems in amorphous materials with arbitrary phonon fields*, Phys. Rev. B **75**, 064202 (2007); cond-mat/0610469.

5. 4. D. V. Anghel, T. Kühn, and Y. M Galperin, *Thermal properties of mesoscopic amorphous membranes*, Series in Micro and Nanotechnologies **11**, 286 (2007).

6. T. Kühn, D. V. Anghel, J. P. Pekola, M. Manninen, and Y. M Galperin, Heat transport in ultra-thin dielectric membranes and bridges, Phys. Rev. B 70, 125425 (2004); cond-mat/0404676.