The investigation of the graphene atom thermal vibrations using forward rainbow scattering

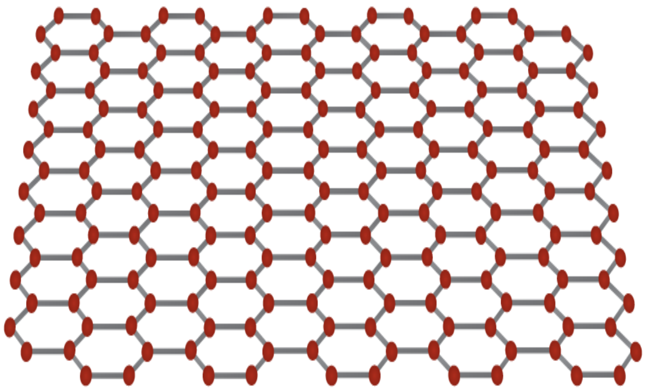
Milivoje Jojić[1], Marko Ćosić[1], Ruslan Rymzhanov[2], Srđan Petrović[1]

[1]Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

[2]Joint Institute for Nuclear Research, Joliot-Curie 6, 141980 Dubna, Moscow Region, Russia

The proton-graphene interaction potential

- We were investigating forward scattering of 5 keV energy protons . Associated proton de Broglie wavelength is $\lambda = 4.0476 \times 10{-}4$ nm , which justifies classical approach.
- Negligible energy loss.
- Neutralization
- The probability density distribution of atom displacements from their equilibrium positions and thermally averaged Doyle-Turner potential are given by following expressions:



Graphene sheet

$$V_{DT}(\boldsymbol{\rho}) = \frac{Z_1 \hbar^2}{4\sqrt{\pi} m_0} \sum_{k=1}^{4} \frac{\alpha_k}{\sqrt{\left|\det \frac{\beta_k}{16\pi^2} \boldsymbol{I}\right|}} \exp\left[-\frac{1}{4} \boldsymbol{\rho}^T \cdot \left(\frac{\beta_k}{16\pi^2} \boldsymbol{I}\right) \cdot \boldsymbol{\rho}\right]$$

$$P_{th}(\boldsymbol{\rho}') = \frac{1}{\sqrt{(2\pi)^3 |\det \boldsymbol{\Sigma}|}} \exp\left[-\frac{1}{2} \boldsymbol{\rho}'^T \cdot \boldsymbol{\Sigma}^{-1} \cdot \boldsymbol{\rho}'\right]$$

$$V_{th}(\boldsymbol{\rho}) = \int_{\boldsymbol{\rho}'} V_{DT}(\boldsymbol{\rho} - \boldsymbol{\rho}') \, P_{th}(\boldsymbol{\rho}') d^3\boldsymbol{\rho}' , \qquad U(\boldsymbol{\rho}) = \sum_i V_{th}(\boldsymbol{\rho} - \boldsymbol{\rho}_i)$$

Rainbow scattering

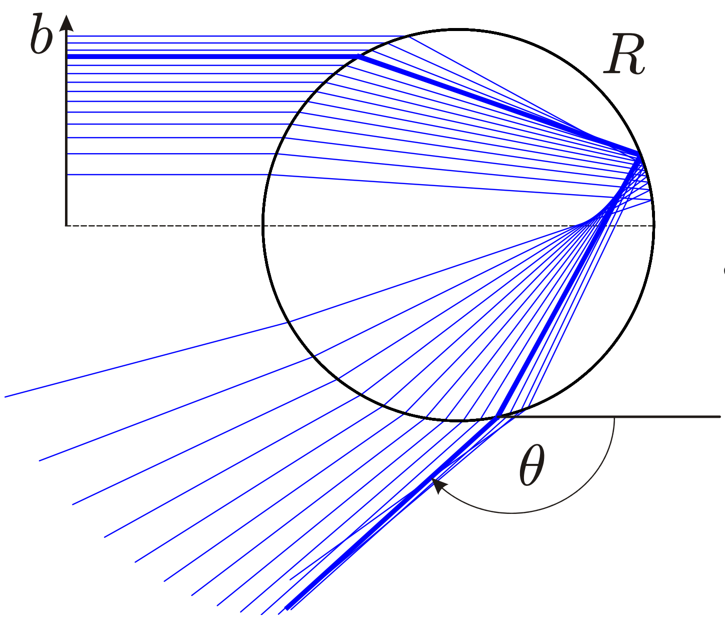
- Equations of motion: $m\frac{d}{dt}\boldsymbol{v} = -\nabla U(\boldsymbol{r})$
- The angular deflection with respect to the incident beam direction is measured by the pair of deflection angles : $\boldsymbol{\theta} = (\theta_x, \theta_y)$, $\tan\theta_x = \frac{v_x}{v_z}$, $\tan\theta_y = \frac{v_y}{v_z}$.
- The differential cross-section :

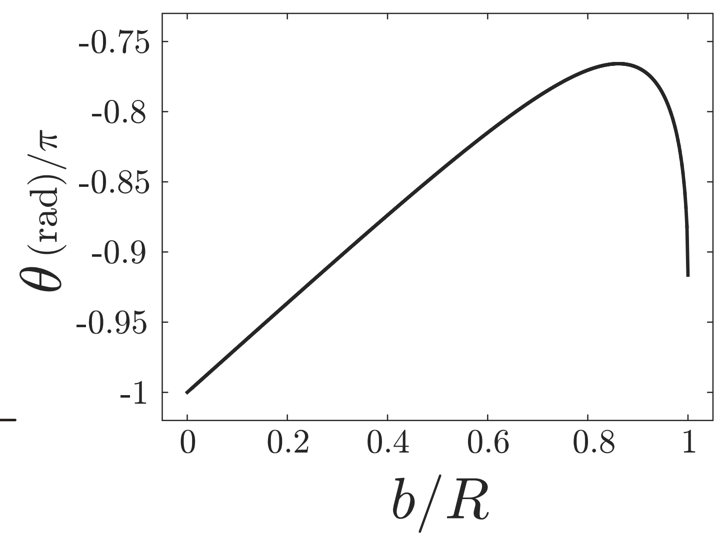
$$\sigma_{\mathrm{diff}}(\boldsymbol{b};\boldsymbol{\Theta},\boldsymbol{\Phi}) \sim \frac{\mathbf{1}}{|\det \boldsymbol{J}_{\boldsymbol{\theta}}(\boldsymbol{b};\boldsymbol{\Theta},\boldsymbol{\Phi})|}$$

In the exit plane the differential cross-section $\sigma_{\mathrm{diff}}(\boldsymbol{b};\boldsymbol{\Theta},\boldsymbol{\Phi})$ is infinite along the lines, called angular rainbow lines.

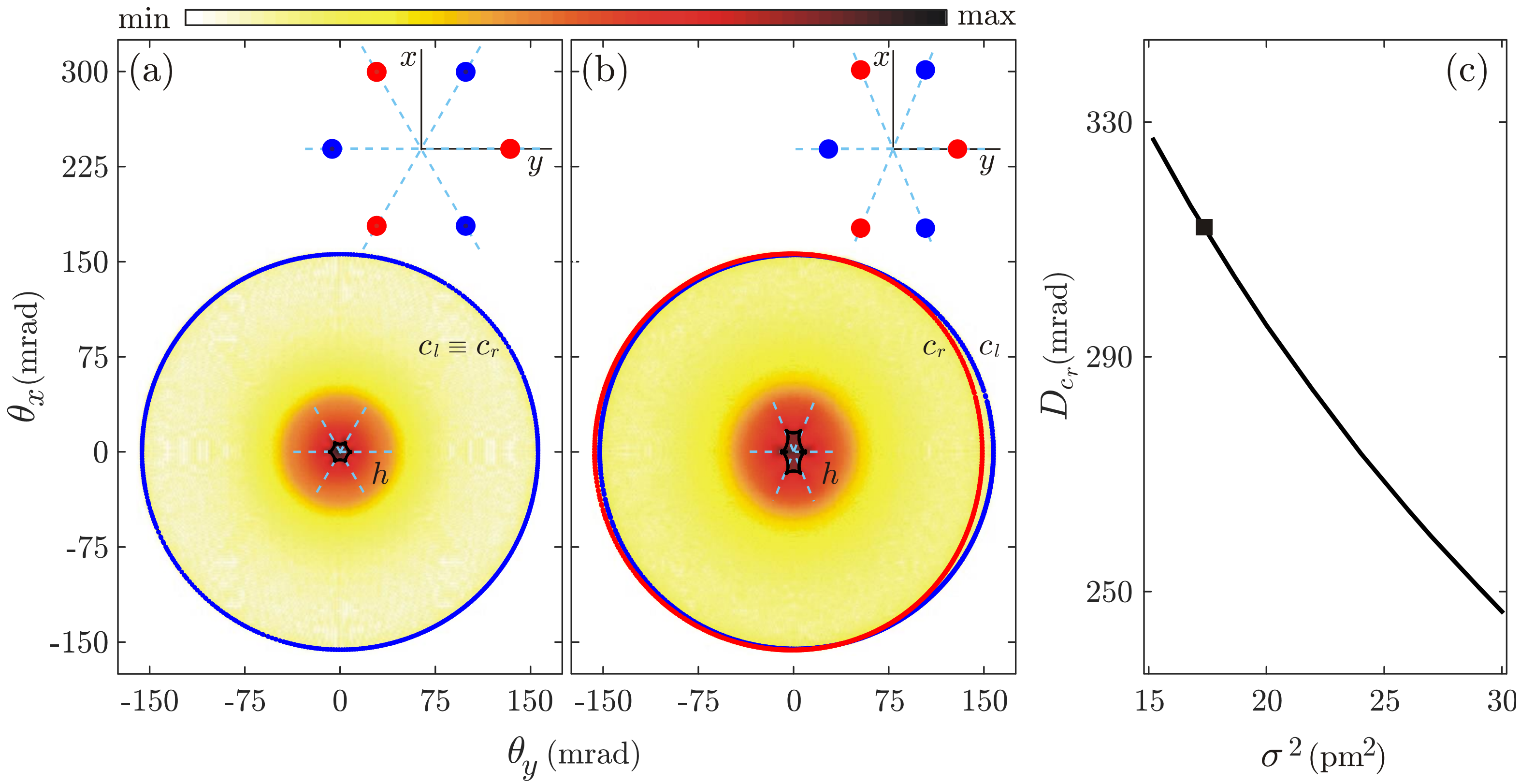
Analogy with light scattering on spherical droplet:

- Relatively large intervals of $\boldsymbol{b}$ are mapped to relatively small intervals of $\boldsymbol{\theta}$ in the vicinities rainbow angles .



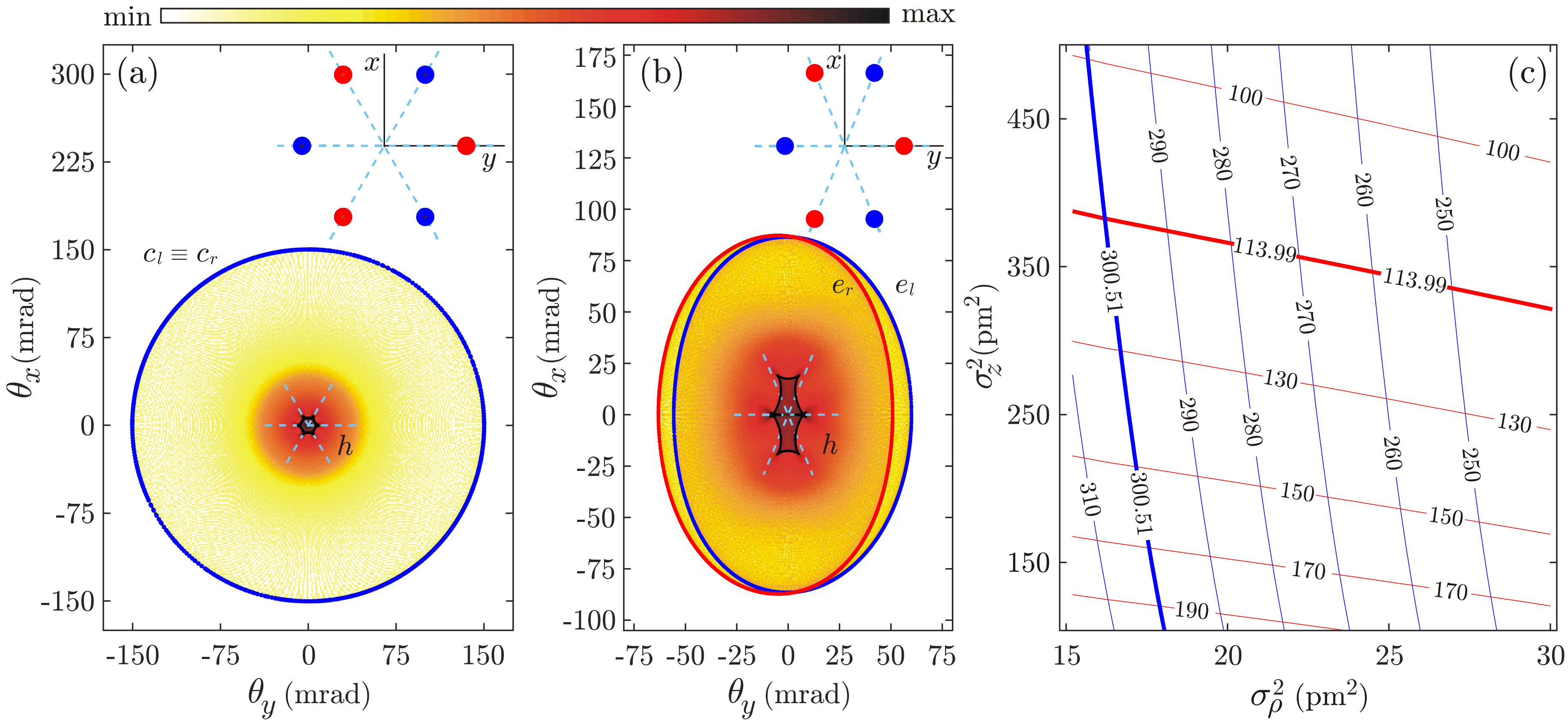


Isotropic thermal vibrations



Graphs: (a) and (b) show angular yields of transmitted protons in logarithmic scale assuming that the incidence angles are 0 rad and $\frac{\pi}{4}$ rad respectively. Corresponding rainbow lines are also shown by black , blue or red doted lines. The relative yield levels are shown by the associated color map. Graph (c) represents calibration curve given as dependence of the diameter of outer rainbow line on variance of thermal vibrations. All shown results corespond to isotropic covariance matrix of the form: $\Sigma = \sigma^2 \cdot 1$.

Anisotropic thermal vibrations



Graphs: (a) and (b) show angular yields in case of when incidence angles are 0 rad and $\frac{\pi}{4}$ rad respectively. Corresponding rainbow lines are also shown by black , blue or red doted lines. Graph (c) shows contour lines in $\left(\sigma_\rho{}^2, \sigma_z{}^2\right)$ plane coresponding to a constant value of diameter of the rainbow line in the normal incidence case and rainbow axis width in θ_y direction in case of $\frac{\pi}{4}$ rad incidence angle , by blue and red colors respectively.

Results corespond to covariance matrix of the form : $\Sigma = diag\ (\sigma_\rho{}^2, \sigma_\rho{}^2, \sigma_z{}^2)$.

Thank you for your attention.

Questions?