



The forward rainbow scattering of low energy protons by a graphene sheet

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ABSTRACT

This article studies the rainbow scattering of 5-keV protons by the single sheet of free-standing graphene and its possible use as a tool for investigation of the ion-graphene interaction. The proton-graphene interaction potential was constructed by using the Doyle-Turner, ZBL, and Molière proton-carbon interaction potentials. The thermal motion of carbon atoms was included by averaging the potentials according to the Debye model. Proton trajectories were obtained by numerical solution of the corresponding Newton equations of motion. They were used to obtain the mapping of the proton initial positions to their scattering angles. Morphological properties of the introduced mapping including its multiplicity and the rainbow singularities were used to explain important features of the obtained angular distributions of transmitted protons.

1. Introduction

Graphene is considered as one of the most promising material in the nano-technological applications nowadays. Probably the best definition of the graphene can be find in Ref. [1] which reads: "Graphene is a single atomic plane of graphite, which is sufficiently isolated from its environment to be considered free-standing". In Ref. [2] its band structure was theoretically investigated almost 70 years ago, however, it was experimentally isolated only recently. Graphene has many interesting physical properties [3]. A lot of them have distinctive topological/morphological origin. Some examples are: the stability of the Dirac cones, the states exhibiting Berry phase of 0 or π rad only, the quantum Hall effect etc. An excellent review of graphene properties from this point of view is presented in Ref. [4].

The rainbow scattering is a physical effect with distinct morphological character too. It occurs when different incoming particles are scattered at the same angle, implying that a mapping of the scattering angles to the particle initial positions is a multi-valued one. The continuity of mapping, on the other hand, guaranties that there are lines in the angular space across which the multiplicity changes discontinuously.

The rainbow effect was observed in many areas of physics. Authors of the Ref. [5] were the first to predict its existence in the semi-classical particle scattering. It was also observed in: nucleus-nucleus collisions [6–8]; electron or ion collisions with atoms or molecules [9,10]; and in the ion scattering from the surfaces [11,12]. The author of the Ref. [13] showed that ion channeling through very thin crystal could be considered as ion scattering through the macro molecule in which the

rainbow scattering occurs. This effect was experimentally verified soon after its prediction [14]. Later it was shown theoretically that the rainbow effect exists also for ions channeling through very short carbon nanotubes [15]. A comprehensive study of rainbows in crystals and carbon nanotubes has been recently published [16]. Aims of the work presented here are to show that the rainbow effect can occur in transmission of protons through a graphene sheet and how this fact can be used as a tool for investigation of the proton-graphene interaction potential.

The central problem in the analysis of ion scattering is the choice of appropriate ion-atom interaction potential. Three commonly used potentials are: Molière [17], Doyle-Turner [18], and Ziegler–Biersack–Littmark (ZBL) [19] potentials. Molières potential is derived from the Thomas–Fermi statistical model of atom, as a simple analytical approximation, where electrons are treated as constituting a free electron gas. It contains no information about the atomic shell structure and because of its statistical nature the difference between model and the actual potential is the largest for the light atoms [20]. However its simple scaling with atomic number makes it still appealing for obtaining basic insight into scattering processes.

The Doyle-Turner's potential is based on the relativistic Hartree–Fock model of atom developed by Grant and Coulthard [21,22]. In this model the magnetic interactions between electrons, retardation effects, finite radius of the nucleus, and all instantaneous correlations in positions of electrons and correlations between electrons of opposite spin are neglected. It was used to calculate spherically symmetrized total charge densities, and atomic potentials of various atoms and ions. Doyle-Turner potentials are the simple analytical

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approximations of these potentials [18]. It is best suited to describe electron-atom or proton-atom collisions.

In the Ziegler–Biersack–Littmark theory interatomic potentials are calculated starting from the spherically symmetrized charge distributions of atoms obtained by the Hartree–Fock approach. The total energy is the sum of the Coulomb interaction energy and a correction required by the Pauli principle due to the overlapping of the electron clouds. Although, the numerical potential is impractical for use in the Monte-Carlo simulations of the atom–atom, and atom-ion collisions, by using a fitting procedure, the authors have found the simple analytical approximation of the universal screening function, with the screening length dependent on atomic numbers of colliding atoms [19]. Introduction of the analytical approximation is motivated by wish to obtain a simple expression for universal nuclear stopping power of reasonable accuracy [19].

Neither potential is able to describe the static polarization effects of electron gas, or corresponding deformations of the electron wavefunctions.

The correct choice of interaction potential is especially important for accurate description of the rainbow channeling effect, where well defined ion trajectory is a consequence of large number of correlated small-angle collisions.

It has been shown that description of the ion-atom interaction by the Molière potential with screening length determined only by target atom atomic number, gives good agreement with the channeling experiments [23]. This was explained by fact that rainbow lines, which dominantly determine the shape of measured distributions, are generated by ions scattering far from atomic strings [24]. Therefore, modification of the screening length, required by formation of the joint electron cloud in the head-on collisions [25], does not influence channeled ions moving far from atomic strings. Resolution and sensitivity of this early experiments were not sufficient for observation of any structure in measured distributions for larger scattering angles. It was observed recently [26] in rainbow channeling of protons in very thin Si crystals, and explained by the rainbow line generated by protons scattered near atomic strings [27]. The analysis have shown that ZBL potential correctly reproduces rainbow lines close to atomic strings while Molière's far from atomic strings [16,28]. Moreover, authors of Refs. [16,28] have shown how rainbow lines can be used for construction of proton-Si interaction potential accurate for all the scattering impact parameters.

In this paper sensitivity of the rainbow lines on small changes of the proton-carbon interaction potential will be demonstrated, proving that rainbow scattering can be a valuable tool for studying the proton-carbon interaction in the graphene.

2. Theory

2.1. Interaction potentials

In our analysis we have applied three commonly used approximations of the proton-carbon interaction potential energy for the construction of the proton-graphene interaction potential energy (the potential shortly further in the text). The first one was Doyle-Turner potential [18]

$$V^{DT}(\boldsymbol{\rho}) \equiv V^{DT}(\rho) = 16\pi^{5/2}Z_1 \frac{\hbar^2}{m} \sum_n \frac{\alpha_n^{DT}}{(\beta_n^{DT})^{3/2}} \exp\left[-4\pi^2 \frac{\rho^2}{\beta_n^{DT}}\right], \quad (1)$$

where $\boldsymbol{\rho}$ is the vector of the proton-carbon distance, $\rho = \|\boldsymbol{\rho}\|$ is its norm, $\alpha^{DT} = (0.07307, 0.1951, 0.04563, 0.01247)$ nm and $\beta^{DT} = (0.369951, 0.112966, 0.028139, 0.003456)$ nm² are Doyle-Turner fitting parameters for carbon atom, \hbar is the reduced Planck constant, m is proton mass and $Z_1 = 1$ is proton atomic number. The second one was ZBL potential [19] which reads

$$V^{ZBL}(\boldsymbol{\rho}) \equiv V^{ZBL}(\rho) = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 \rho} \sum_n \alpha_n^{ZBL} \exp\left[-\beta_n^{ZBL} \frac{\rho}{a_{ZBL}}\right], \quad (2)$$

where $\alpha^{ZBL} = (0.1818, 0.5099, 0.2802, 0.02817)$ and $\beta^{ZBL} = (3.2, 0.9423, 0.4029, 0.2016)$ are the ZBL fitting parameters, ϵ_0 is the vacuum permittivity, $Z_2 = 6$ is carbon atomic number, $e = 1.6 \cdot 10^{-19}$ C is the elementary charge, $a_{ZBL} = (9\pi^2/128)^{1/3} / (Z_1^{0.23} + Z_2^{0.23}) a_0$ is the screening radius and $a_0 = 0.0529$ nm is the Bohr radius. The third one was the Molière potential $V^M(\boldsymbol{r})$ [17] which is given by the equation completely similar to the Eq. (2) in which α^{ZBL} and β^{ZBL} were substituted with the Molière fitting parameters $\alpha^M = (0.35, 0.55, 0.10)$ and $\beta^M = (0.1, 1.2, 6.0)$, while a_Z needs to be substituted with the Firsov screening radius $a_F = (9\pi^2/128)^{1/3} / (Z_1^{1/2} + Z_2^{1/2})^{3/2} a_0$ [25].

It has been assumed that thermal vibrations of the carbon atoms in the graphene are random, isotropic, uncorrelated and that can be adequately described by the Debye model [29,30]. The probability density distribution of atom displacements from their equilibrium positions reads

$$P_{th}(\boldsymbol{\rho}') = \frac{1}{(2\pi\sigma_{th}^2)^{3/2}} \exp\left[-\frac{\|\boldsymbol{\rho}'\|^2}{2\sigma_{th}^2}\right], \quad (3)$$

with a root-mean-square (RMS) value of displacements

$$\sigma_{th} = \frac{3^{1/2}\hbar}{(M_c m_u k_B \Theta_D)^{1/2}} \left(\frac{D_f(T/\Theta_D)}{T/\Theta_D} + \frac{1}{4}\right)^{1/2}, \quad (4)$$

where $M_c = 12.01$ is carbon atomic weight, $m_u = 1.6605 \cdot 10^{-27}$ kg is universal atomic mass unit, $\Theta_D = 2000$ K is the carbon Debye temperature, $k_B = 1.3806 \cdot 10^{-23}$ J/K is Boltzman's constant, T is the graphene absolute temperature, and D_f is the Debye's function. The thermally averaged potential is then given by the expression

$$V_{th}(\boldsymbol{\rho}) = \int_{\boldsymbol{\rho}'} V(\boldsymbol{\rho} - \boldsymbol{\rho}') P_{th}(\boldsymbol{\rho}') d^3\rho'. \quad (5)$$

For considered potentials the integral (5) can be evaluated analytically. The straightforward evaluation shows that the thermally averaged Doyle-Turner potential $V_{th}^{DT}(\boldsymbol{\rho})$ can be obtained from the Eq. (1) if β_n^{DT} is substituted by $\bar{\beta}_n^{DT} = \beta_n^{DT} + 8\pi^2\sigma_{th}^2$. The thermally averaged ZBL potential $V_{th}^{ZBL}(\boldsymbol{\rho})$ reads

$$V_{th}^{ZBL}(\boldsymbol{\rho}) \equiv V_{th}^{ZBL}(\rho) = \frac{Z_1 Z_2 e^2}{8\pi\epsilon_0 \rho} \sum_n \alpha_n^{ZBL} \exp\left[\left(\frac{\beta_n^{ZBL} \sigma_{th}}{\sqrt{2} a_{ZBL}}\right)^2\right] \left\{ \exp\left(-\frac{\beta_n^{ZBL} \rho}{a_{ZBL}}\right) \operatorname{erfc}\left(\frac{\beta_n^{ZBL} \sigma_{th}}{\sqrt{2} a_{ZBL}} - \frac{\rho}{\sqrt{2} \sigma_{th}}\right) - \exp\left(\frac{\beta_n^{ZBL} \rho}{a_{ZBL}}\right) \operatorname{erfc}\left(\frac{\beta_n^{ZBL} \sigma_{th}}{\sqrt{2} a_{ZBL}} + \frac{\rho}{\sqrt{2} \sigma_{th}}\right) \right\} \quad (6)$$

where erfc stands for the complementary error function [31]. The thermally averaged Molière's potential $V_{th}^M(\boldsymbol{\rho})$ is given by the same Eq. (6) in which fitting parameters α^{ZBL} , β^{ZBL} , and a_{ZBL} are substituted by α_M , β_M , and a_F respectively.

The proton-graphene potential is the sum of the proton-carbon potentials that contribute to the scattering process. This sum should resemble the graphene's geometric structure and its symmetry. The graphene posses the translational symmetry with the rhombic Bravais lattice, defined by the primitive vectors $\mathbf{a}_1 = (\sqrt{3}l/2, 3l/2, 0)$ and $\mathbf{a}_2 = (-\sqrt{3}l/2, 3l/2, 0)$, where $l = 0.144$ nm is the carbon–carbon bond length. The repeating motif consists of two carbon atoms whose positions relative to the vertices of the unit cells are $\mathbf{g}_1 = (-l/2, 0, 0)$ and $\mathbf{g}_2 = (l/2, 0, 0)$. This specific values of vectors \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{g}_1 , and \mathbf{g}_2 result in the C_{6v} point group symmetry relative to the center of graphene's hexagon [4]. If the coordinate origin is set to the most symmetric point (the center of the hexagon), then the graphene potential reads

$$U(\mathbf{r}) = \sum_{n_1, n_2} \sum_k V_{th}(\|\mathbf{r} + \mathbf{g}_k + (n_1 - 1/2)\mathbf{a}_1 + (n_2 - 1/2)\mathbf{a}_2\|), \quad (7)$$

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