



## The donut and dynamic polarization effects in proton channeling through carbon nanotubes

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## The donut and dynamic polarization effects in proton channeling through carbon nanotubes

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**Abstract.** We investigate the angular and spatial distributions of protons with an energy of 0.223 MeV after channeling them through an (11, 9) single-wall carbon nanotube of 0.2  $\mu\text{m}$  length. The proton incident angle is varied between 0 and 10 mrad, being close to the critical angle for channeling. We show that, as the proton incident angle increases and approaches the critical angle for channeling, a ring-like structure is developed in the angular distribution—the donut effect. We demonstrate that it is the rainbow effect. If the proton incident angle is between zero and half of the critical angle for channeling, the image force affects considerably the number and positions of the maxima of the angular and spatial distributions. However, if the proton incident angle is close to the critical angle for channeling, its influence on the angular and spatial distributions is considerably decreased. We demonstrate that an increase of the proton incident angle can lead to a significant rearrangement of the propagating protons within the nanotube. This effect may be used to locate atomic impurities in nanotubes as well as for creating nanosized proton beams to be used in materials science, biology and medicine.

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**Contents**

<b>1. Introduction</b>	<b>2</b>
<b>2. Theory</b>	<b>3</b>
<b>3. Results and discussion</b>	<b>5</b>
<b>4. Concluding remarks</b>	<b>15</b>
<b>Acknowledgments</b>	<b>15</b>
<b>References</b>	<b>15</b>

**1. Introduction**

While the progress in theoretical modeling and computer simulation of ion channeling through carbon nanotubes has reached an advanced level, as reviewed in [1–10], the experimental advancement in this area is still in its infancy. Since the issues of ordering, straightening and holding nanotubes are probably the most challenging tasks in the experimental realization of ion channeling through them, it is not surprising that the best results in performing these tasks can be expected when they are grown in a dielectric medium. For example, the first experimental data on ion channeling through nanotubes, reported by Zhu *et al* [11], were obtained with He<sup>+</sup> ions and an array of well-ordered multi-wall nanotubes grown in a porous anodic aluminum oxide (Al<sub>2</sub>O<sub>3</sub>) membrane. Zhu *et al* performed direct measurements of the yield of ions transmitted through a bare Al<sub>2</sub>O<sub>3</sub> sample and an Al<sub>2</sub>O<sub>3</sub> sample with nanotubes and then compared the results for the two samples.

On the other hand, the first experimental results on electron channeling through carbon nanotubes have been reported by Chai *et al* [12]. The authors studied the transport of electrons with an energy of 300 keV through aligned multi-wall nanotubes of 0.7–3.0  $\mu\text{m}$  length embedded in carbon fiber coatings. The misalignment of the nanotubes was up to 1°. Besides, Berdinsky *et al* [13] have succeeded in growing single-wall carbon nanotubes (SWCNTs) in ion tracks etched in SiO<sub>2</sub> layers on an Si substrate, offering the interesting possibility of experimental realization of ion channeling through nanotubes in a wide range of ion energies.

Regarding the theoretical modeling and computer simulation of ion channeling through carbon nanotubes, we note that the effect of dynamic polarization of the nanotube atoms' valence electrons by the ion is not usually taken into account [1–14], since its influence at very low and very high energies, of the order of 1 keV and 1 GeV, respectively, is negligible. However, it is expected that at medium energies, of the order of 1 MeV, this effect contributes significantly to the ion energy loss and gives rise to an additional force acting on the ions, called the image force [15, 16], as it has been demonstrated in the computer simulation of the angular distributions of protons channeled through SWCNTs in vacuum [17]. The importance of the image force has also been emphasized in the related area of ion transmission through cylindrical channels in metals [18–23] and on ions and molecules moving over supported graphene [24, 25].

As far as the ion channeling dynamics at very low and very high energies is concerned, the material surrounding the carbon nanotubes serves predominantly as their passive container. However, the ions moving at medium energies induce a strong dynamic polarization of both, the nanotube atoms' valence electrons and the surrounding material, which in turn gives rise to a sizeable image force [26, 27]. In these two studies, the image force was calculated by

a two-dimensional (2D) hydrodynamic model of the nanotube atoms' valence electrons, while the surrounding material was described by a frequency-dependent dielectric function. On the other hand, the image force has recently been shown to influence significantly the rainbow effect in proton channeling through the short SWCNTs [28] and double-wall nanotubes in vacuum [29] as well as through the short SWCNTs in the dielectric media [30, 31]. We believe that it is important to improve our understanding of the role of the image force in the rainbow effect with nanotubes because, in analogy with the case of surface ion channeling [32–34], measurements of this effect can give precise information on both the atomic configuration and interaction potentials within nanotubes, which have not yet been explored completely.

However, in ion channeling experiments, the always present questions are the ones of ion beam divergence and misalignment. So, it is important to study the influence of the effect of dynamic polarization of carbon nanotubes when the initial ion velocity is not parallel to the nanotube axis. Therefore, in this paper, we continue our investigation of the image force for the case where the ion incident angle is not zero. Specifically, we analyze the angular and spatial distributions of protons with a velocity of 3 a.u. channeled through straight (11, 9) SWCNTs of  $0.2 \mu\text{m}$  length in vacuum. The proton incident angle is varied between 0 and 10 mrad, being close to the critical angle for channeling. This proton velocity is chosen because the dynamic polarization effect is strongest in the range around it. The consideration is limited to the case of a nanotube in vacuum because the presence of a dielectric medium around it would introduce only a slight modifying factor in the results of calculation [30, 31].

It is well known that, for ion incident angles close to the critical angle for channeling, the donut effect develops in the angular distributions of channeled ions. The effect was measured with Si and Ge crystals [35–37], and explained independently afterwards by the theory of crystal rainbows [38, 39]. That theory was formulated as a proper theory of ion channeling through thin crystals [40], and has been applied subsequently to ion channeling through short carbon nanotubes [41–44]. It must be noted that the donut effect has also been observed in a computer simulation of ion propagation through nanotubes [45]. However, the authors did not connect the obtained results to the rainbow effect. We explore here the donut effect in the angular and spatial distributions of protons channeled through an (11, 9) SWCNT in the presence of the image force.

Regarding the angular and spatial distributions of channeled protons to be presented in this study, corresponding to the case where the proton incident angle is not zero, we note that the proton equations of motion in the transverse position plane that are solved to generate them are 2D. This means that the case we explore is truly 2D, unlike the cases treated in our previous studies of the image force in carbon nanotubes, which were in fact 1D [28–31].

Atomic units will be used throughout the paper unless explicitly stated otherwise.

## 2. Theory

We adopt the right Cartesian coordinate system with the  $z$ -axis coinciding with the nanotube axis, the origin in the entrance plane of the nanotube, and the  $x$ - and  $y$ -axes the vertical and horizontal axes, respectively. The initial proton velocity,  $\vec{v}$ , is taken to lie in the  $yz$ -plane and make angle  $\varphi$  with the  $z$ -axis, being the proton incident angle. The length of the nanotube,  $L$ , is assumed to be large enough to allow us to ignore the influence of the nanotube edges on the image force and, at the same time, small enough to neglect the energy losses of channeled protons.

We assume that the interaction between the proton and nanotube atoms can be treated classically using the Doyle–Turner expression [46] averaged axially [47] and azimuthally [45]. This interaction is repulsive and of short-range character. Thus, the repulsive interaction potential in the proton channeling through the nanotube is of the form

$$U_{\text{rep}}(r) = \frac{32\pi d Z_1 Z_2 a}{3\sqrt{3}l^2} \sum_{j=1}^4 a_j b_j^2 I_0(2ab_j^2 r) \exp\{-b_j^2[r^2 + a^2]\}, \quad (1)$$

where  $Z_1 = 1$  and  $Z_2 = 6$  are the atomic numbers of the hydrogen and carbon atoms, respectively,  $a$  is the nanotube radius,  $l$  is the nanotube atoms' bond length,  $r = (x^2 + y^2)^{1/2}$  is the distance between the proton and the nanotube axis,  $I_0$  is the modified Bessel function of the first kind and zeroth order, and  $a_j = \{0.115, 0.188, 0.072, 0.020\}$  and  $b_j = \{0.547, 0.989, 1.982, 5.656\}$  are the fitting parameters (in atomic units) [46].

The dynamic polarization of the nanotube by the proton is treated via a 2D hydrodynamic model of the nanotube atoms' valence electrons, based on a jellium-like description of the ion cores making the nanotube wall [15–26]. This model includes the axial and azimuthal averaging similar to that applied in obtaining the corresponding repulsive interaction potential, given by equation (1). It finally gives the interaction potential between the proton and its image,  $U_{\text{im}}(r, t)$ , which is stationary in the coordinate system moving with the proton and depends on its velocity. This interaction is attractive and of long-range character. The details of derivation of the expression for  $U_{\text{im}}(r, t)$  are given elsewhere [15–30]. Consequently, the total interaction potential in the proton channeling through the nanotube is

$$U(r, t) = U_{\text{rep}}(r) + U_{\text{im}}(r, t). \quad (2)$$

The proton equations of motion we solve are

$$m\ddot{x}(t) = -\frac{\partial U(r, t)}{\partial x}, \quad (3)$$

$$m\ddot{y}(t) = -\frac{\partial U(r, t)}{\partial y}, \quad (4)$$

where  $m$  is the proton mass. They are subject to the initial conditions for the transverse components of the proton velocity namely,

$$\dot{x}(t = 0) = 0, \quad (5)$$

$$\dot{y}(t = 0) = v \sin \varphi \approx v\varphi. \quad (6)$$

The longitudinal proton motion is treated as uniform with the initial condition for the longitudinal component of the proton velocity, namely  $\dot{z}(t = 0) = v \cos \varphi \approx v$ . As a result, the longitudinal component of the proton position is  $z(t) = vt$ . Equations (5) and (6) are solved numerically. The angular and spatial distributions of transmitted protons are generated using a Monte Carlo computer simulation code. The components of the proton impact parameter,  $x_0$  and  $y_0$ , are chosen randomly from a uniform distribution within the cross-sectional area of the nanotube and its entrance plane. With  $l = 0.144$  nm [48], we obtain that  $a = 0.689$  nm. If the proton impact parameter falls inside the annular interval  $[a - a_{\text{sc}}, a]$ , where  $a_{\text{sc}} = [9\pi^2/(128Z_2)]^{1/3}a_0$  is the screening radius and  $a_0$  the Bohr radius, the proton is treated as if it is backscattered and is disregarded. The initial number of protons is about 1000 000.

The components of the proton scattering angle,  $\Theta_x$  and  $\Theta_y$ , are obtained via expressions  $\Theta_x = V_x/v$  and  $\Theta_y = V_y/v$ , where  $V_x$  and  $V_y$  are the final transverse components of the proton velocity, which are obtained, together with the final transverse components of the proton position,  $X$  and  $Y$ , as the solutions of equations (5) and (6). The proton channeling through the nanotube can be analyzed via the mapping of the impact parameter plane, the  $x_0y_0$  plane, to the scattering angle plane, the  $\Theta_x\Theta_y$  plane [40]. The corresponding total interaction potential, given by equation (2), is axially symmetric. This means that if the initial proton velocities were parallel to the nanotube axis, this mapping would be 1D. However, the initial proton velocities are not parallel to the nanotube axis, and the mapping is 2D. Since the proton scattering angle is small, its differential transmission cross section is given by

$$\sigma = -\frac{1}{|J_{\Theta}|}, \quad (7)$$

where  $J_{\Theta}$  is the Jacobian of the mapping,

$$J_{\Theta} = \frac{\partial\Theta_x}{\partial x_0} \frac{\partial\Theta_y}{\partial y_0} - \frac{\partial\Theta_x}{\partial y_0} \frac{\partial\Theta_y}{\partial x_0}. \quad (8)$$

Thus, the equation  $J_{\Theta} = 0$  determines the lines in the impact parameter plane along which the proton differential transmission cross section is singular. The images of these lines in the scattering angle plane are the rainbow lines in this plane [40].

We can analyze in a similar way the mapping of the impact parameter plane (the  $x_0y_0$  plane), which is the entrance plane of the nanotube and the initial transverse position plane, to the exit plane of the nanotube or the final transverse position plane, the  $XY$  plane. The Jacobian of this mapping is

$$J_R = \frac{\partial X}{\partial x_0} \frac{\partial Y}{\partial y_0} - \frac{\partial X}{\partial y_0} \frac{\partial Y}{\partial x_0}. \quad (9)$$

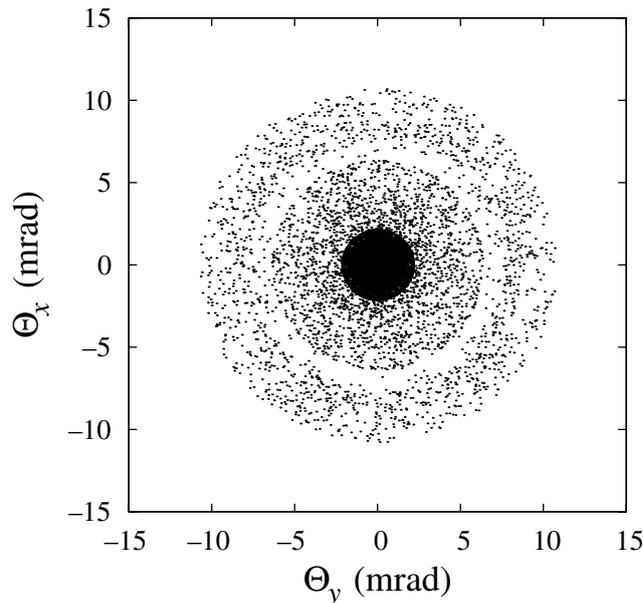
The rainbow lines in the final transverse position plane are the images of the lines in the impact parameter plane determined by the equation  $J_R = 0$ .

### 3. Results and discussion

Let us now analyze the angular and spatial distributions of protons channeled in the (11, 9) SWCNT of  $0.2 \mu\text{m}$  length. In all the cases to be studied, the initial proton velocity will be  $v = 3 \text{ a.u.}$ , corresponding to the initial proton energy of  $0.223 \text{ MeV}$ , while the incident proton angle,  $\varphi$ , will be varied between  $0$  and  $10 \text{ mrad}$ . The maximal proton incident angle will be close to the critical angle for channeling,  $\psi_c$ , being about  $11 \text{ mrad}$ . The analysis will also include the typical proton trajectories through the nanotube in the proton phase space.

In figures 1–6, we shall display the evolution of the angular distribution of channeled protons with the increase of  $\varphi$ . In particular, we shall analyze the development of a ring-like structure in the angular distribution under the influence of the image force.

The scatter plot shown in figure 1 represents the angular distribution of channeled protons for  $\varphi = 0$  with the image force included. The corresponding angular distribution without the inclusion of the image force contains in its central part only a maximum at the origin. This means that the non-monotonic character of the central part of the angular distribution with the image force included is due to the effect of dynamic polarization. This was discussed in one of our previous papers [28]. We presented in it the distributions of channeled protons along

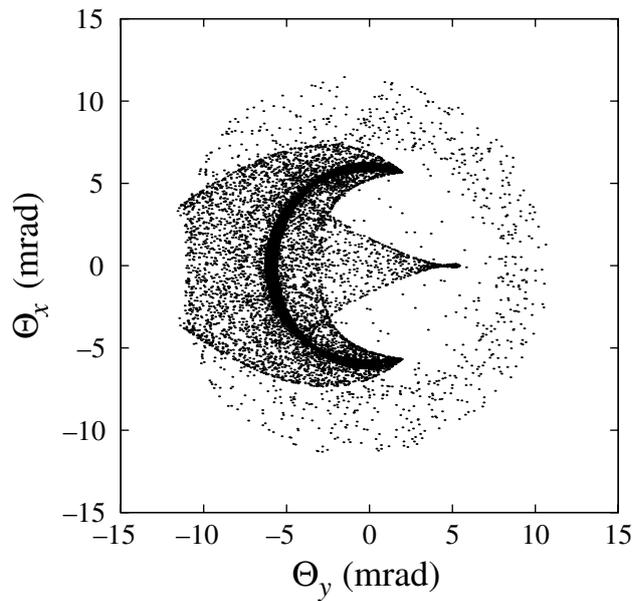


**Figure 1.** The angular distribution of protons channeled in the (11, 9) SWCNT with the inclusion of the image force when the proton incident angle  $\varphi = 0$ . The proton velocity is  $v = 3$  a.u., the nanotube radius  $a = 0.689$  nm and the nanotube length  $L = 0.2 \mu\text{m}$ .

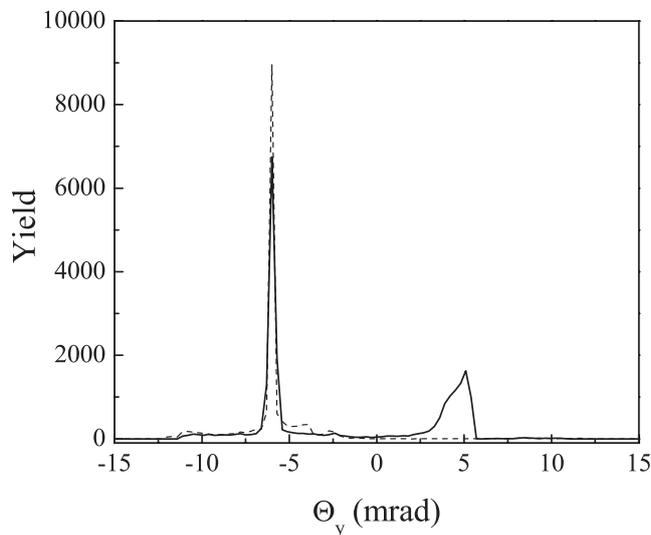
the  $\Theta_y$ -axis (in the scattering angle plane) with and without the image force included, which were in fact (for  $\varphi = 0$ ) the radial yields of channeled protons. The conclusion of the discussion was that the maxima of the radial yield, appearing when the image force was included, were due to the rainbow effect.

Figure 2 gives the angular distribution of channeled protons for  $\varphi = 6$  mrad with the image force included. The angular distribution is characterized with a half of a ring-like structure, with an exceptionally high yield of channeled protons. This is the precursor of the effect known as the donut effect, which is connected to the misalignment of the proton beam and nanotube axis. In addition, the angular distribution contains several intricately shaped regions with lower yields of channeled protons. We show in figure 3 the corresponding distribution of channeled protons along the  $\Theta_y$ -axis with and without the image force included. The sharp maximum of this distribution, appearing at  $-6.0$  mrad, is due to the donut effect. It is evident that the image force makes this maximum weaker. On the other hand, the origin of the broad maximum of the distribution, located at  $-5.1$  mrad, is solely the image force. Thus, we can conclude that for the median values of  $\varphi$ , between 0 and about  $\psi_c/2$ , the image force still plays a significant role in generating the angular distribution.

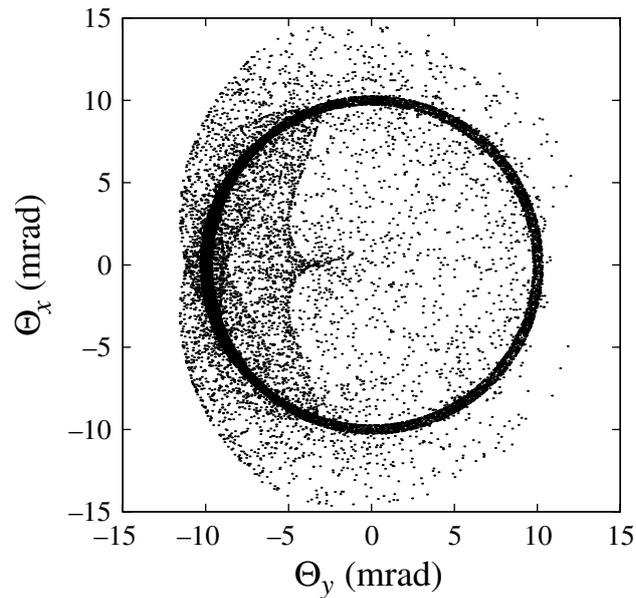
We show in figure 4 the angular distribution of channeled protons for  $\varphi = 10$  mrad with the image force included. One can clearly see the whole ring-like structure, with an exceptionally high yield of channeled protons. This is the fully developed donut effect. As it has been already said, the corresponding value of  $\varphi$  is close to the value of  $\psi_c$ . In addition, as in figure 2, the angular distribution contains several intricately shaped regions with lower but distinctly graded yields of channeled protons, with very clear boundaries between them. Figure 5 gives the corresponding distribution of channeled protons along the  $\Theta_y$ -axis with and without the



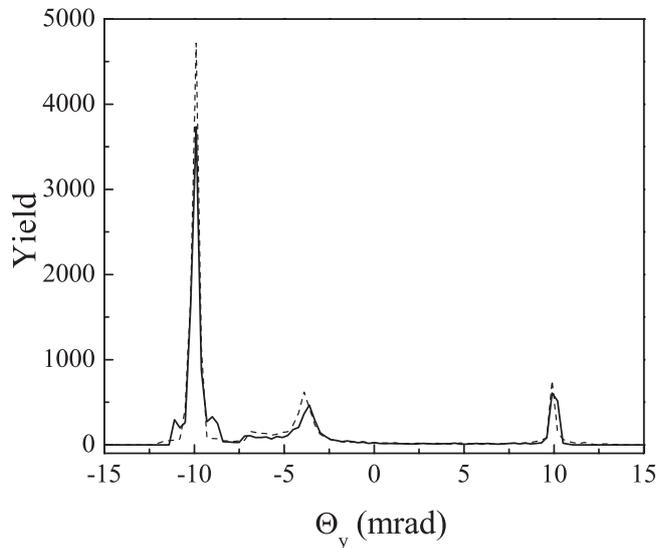
**Figure 2.** The angular distribution of protons channeled in the (11, 9) SWCNT with the inclusion of the image force when the proton incident angle  $\varphi = 6$  mrad. The proton velocity is  $v = 3$  a.u., the nanotube radius  $a = 0.689$  nm and the nanotube length  $L = 0.2 \mu\text{m}$ .



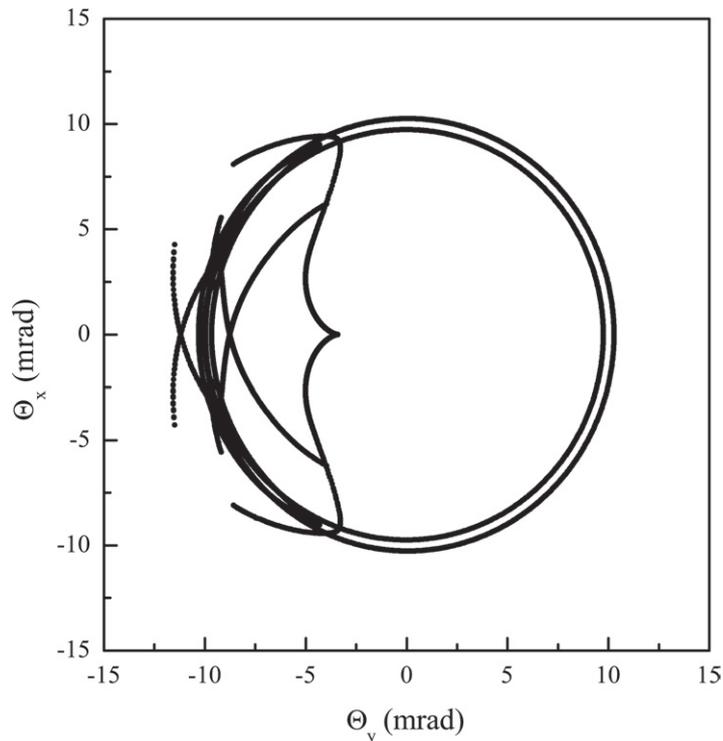
**Figure 3.** The distribution along the  $\Theta_y$ -axis of protons channeled in the (11, 9) SWCNT with the image force taken into account—the solid curve—and without it—the dashed curve—when the proton incident angle  $\varphi = 6$  mrad. The proton velocity is  $v = 3$  a.u., the nanotube radius  $a = 0.689$  nm and the nanotube length  $L = 0.2 \mu\text{m}$ . The former curve corresponds to the angular distribution shown in figure 2.



**Figure 4.** The angular distribution of protons channeled in the (11, 9) SWCNT with the inclusion of the image force when the proton incident angle  $\varphi = 10$  mrad. The proton velocity is  $v = 3$  a.u., the nanotube radius  $a = 0.689$  nm and the nanotube length  $L = 0.2 \mu\text{m}$ .



**Figure 5.** The distribution along the  $\Theta_y$ -axis of protons channeled in the (11, 9) SWCNT with the image force taken into account—the solid curve—and without it—the dashed curve—when the proton incident angle  $\varphi = 10$  mrad. The proton velocity is  $v = 3$  a.u., the nanotube radius  $a = 0.689$  nm and the nanotube length  $L = 0.2 \mu\text{m}$ . The former curve corresponds to the angular distribution shown in figure 4.



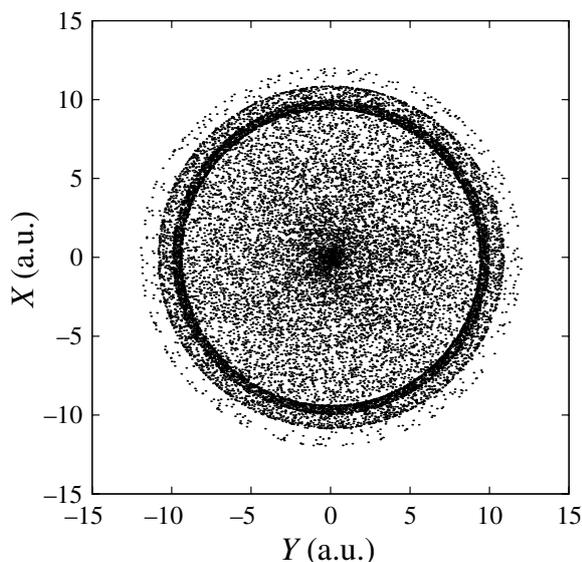
**Figure 6.** The rainbow lines in the scattering angle plane for the protons channeled in the (11, 9) SWCNT with the inclusion of the image force when the proton incident angle  $\varphi = 10$  mrad. The proton velocity is  $v = 3$  a.u., the nanotube radius  $a = 0.689$  nm and the nanotube length  $L = 0.2$   $\mu\text{m}$ .

image force included. It is evident that, when  $\varphi$  is close to  $\psi_c$ , the role of the effect of dynamic polarization in generating the angular distribution is almost negligible. Figure 6 shows the corresponding rainbow lines in the scattering angle plane with the dynamic polarization effect taken into account. These lines clearly demonstrate that the non-uniformity of the angular distribution, including the donut effect, is due to the rainbow effect.

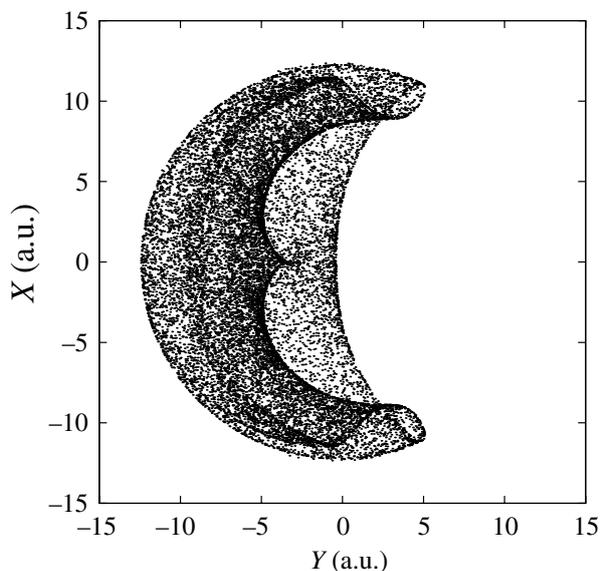
In figures 7–10, we shall display the evolution of the spatial distribution of channeled protons with the increase of  $\varphi$ , which is going on in parallel with the evolution of the angular distribution displayed in figures 1–6.

The scatter plot given in figure 7 represents the spatial distribution of channeled protons for  $\varphi = 0$  with the image force included. This spatial distribution and the corresponding spatial distribution without the image force included were analyzed in one of our previous papers [31]. We presented in it the distributions of channeled protons along the  $y$ -axis with and without the image force included, which were in fact (for  $\varphi = 0$ ) the radial yields of channeled protons. It was demonstrated that the maxima of the radial yields, present in both spatial distributions, were the rainbow maxima. We also concluded that the dynamic polarization effect caused the shifts of the maxima of the spatial distribution generated with the effect not taken into account as well as the appearance of additional maxima.

The spatial distribution of channeled protons for  $\varphi = 10$  mrad with the effect of dynamic polarization taken into account is presented in figure 8. When this spatial distribution is

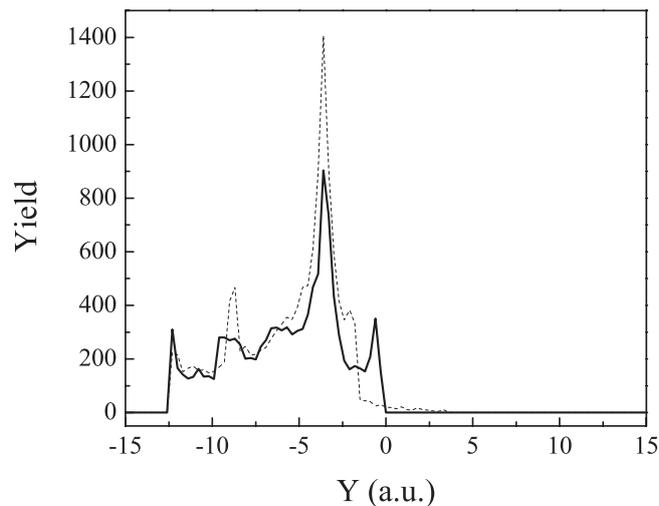


**Figure 7.** The spatial distribution of protons channeled in the (11, 9) SWCNT with the image force included when the proton incident angle  $\varphi = 0$ . The proton velocity is  $v = 3$  a.u., the nanotube radius  $a = 0.689$  nm and the nanotube length  $L = 0.2$   $\mu\text{m}$ .



**Figure 8.** The spatial distribution of protons channeled in the (11, 9) SWCNT with the inclusion of the image force when the proton incident angle  $\varphi = 10$  mrad. The proton velocity is  $v = 3$  a.u., the nanotube radius  $a = 0.689$  nm and the nanotube length  $L = 0.2$   $\mu\text{m}$ .

compared with the spatial distribution for  $\varphi = 0$ , it is evident that the maximal change of  $\varphi$  induces a significant rearrangement of the protons in the final transverse position plane. Almost all the protons are displaced to the left half of the nanotube. However, as in the cases



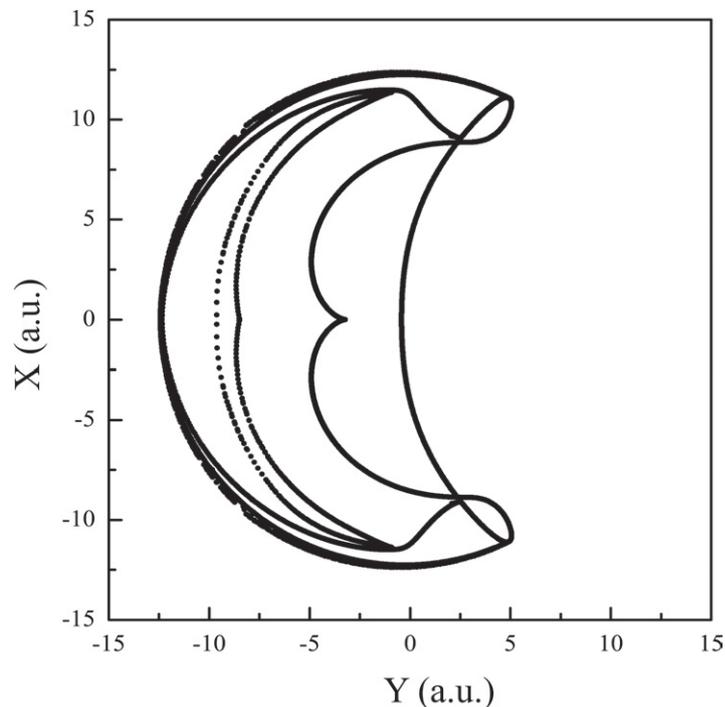
**Figure 9.** The distribution along the  $Y$ -axis of protons channeled in the (11, 9) SWCNT with the image force taken into account—the solid curve—and without it—the dashed curve—when the proton incident angle  $\varphi = 10$  mrad. The proton velocity is  $v = 3$  a.u., the nanotube radius  $a = 0.689$  nm and the nanotube length  $L = 0.2$   $\mu\text{m}$ . The former curve corresponds to the spatial distribution given in figure 8.

of angular distributions for  $\varphi = 6$  and 10 mrad, the spatial distribution also contains several intricately shaped regions with lower but distinctly graded yields of channeled protons, with very clear boundaries between them. Figure 9 gives the corresponding distribution of channeled protons along the  $Y$ -axis, in the final transverse position plane, with and without the image force included. For this value of  $\varphi$ , the strongest maximum of the spatial distribution lies at  $-3.6$  a.u. instead of at the origin for  $\varphi = 0$ . One can also conclude that, when  $\varphi$  is close to  $\psi_c$ , the role of the effect of dynamic polarization in generating the spatial distribution is small but noticeable. The effect makes the strongest maximum of the spatial distribution weaker and induces a rightward shift of the second strongest maximum. Figure 10 shows the corresponding rainbow lines in the final transverse position plane with the image force taken into account. As in the case of angular distribution for this value of  $\varphi$ , these lines clearly demonstrate that the non-uniformity of the spatial distribution is to be attributed to the rainbow effect.

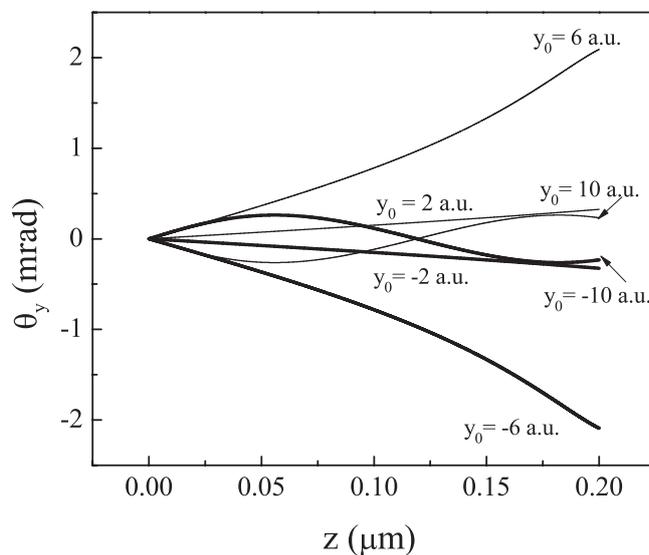
In figures 11–14, we shall display the typical proton trajectories through the nanotube in the proton phase space, complementing the result displayed in figures 1–10.

We show in figure 11 the  $y$ -component of the proton scattering angle ( $\Theta_y$ ) as a function of the  $z$ -component of its position within the nanotube with the effect of dynamic polarization included when  $\varphi = 0$  for  $x_0 = 0$  and  $y_0 = \pm 2, \pm 6$  and  $\pm 10$  a.u. Looking at the angular distribution shown in figure 1, we see that the channeled protons with the impact parameters close to the nanotube axis, i.e. for  $y_0 = \pm 2$  a.u., and close to the nanotube wall, i.e. for  $y_0 = \pm 10$  a.u., contribute to the part of the angular distribution close to the origin. The channeled protons with the impact parameters comparable with  $a/2$ , i.e. for  $y_0 = \pm 6$  a.u., give rise to the rainbow maxima lying at about 2 mrad.

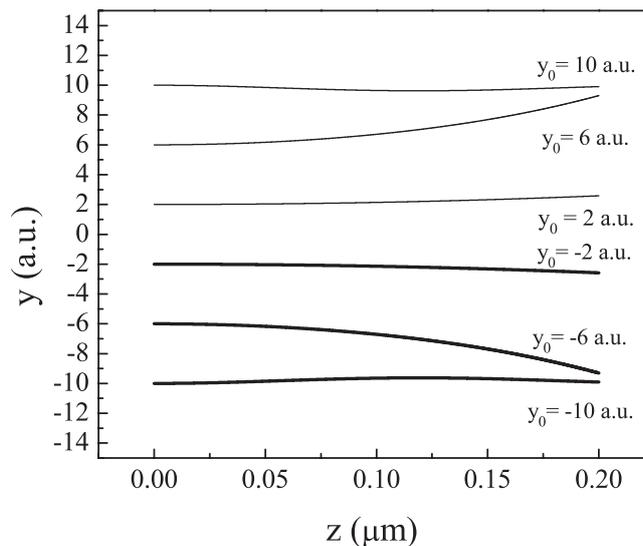
Figure 12 gives the dependence of the  $y$ -component of the proton position on the  $z$ -component of its position within the nanotube with the image force included when  $\varphi = 0$  for



**Figure 10.** The rainbow lines in the final transverse position plane for the protons channeled in the (11, 9) SWCNT with the image force included when the proton incident angle  $\varphi = 10$  mrad. The proton velocity is  $v = 3$  a.u., the nanotube radius  $a = 0.689$  nm and the nanotube length  $L = 0.2$   $\mu\text{m}$ .



**Figure 11.** The dependence of the  $y$ -component of the proton scattering angle on the  $z$ -component of its position in the channeling through the (11, 9) SWCNT with the inclusion of the image force when the proton incident angle  $\varphi = 0$  for the  $x$ -component of the proton impact parameter  $x_0 = 0$  and the  $y$ -component of its impact parameter  $y_0 = \pm 2, \pm 6$  and  $\pm 10$  a.u. The proton velocity is  $v = 3$  a.u., the nanotube radius  $a = 0.689$  nm and the nanotube length  $L = 0.2$   $\mu\text{m}$ .



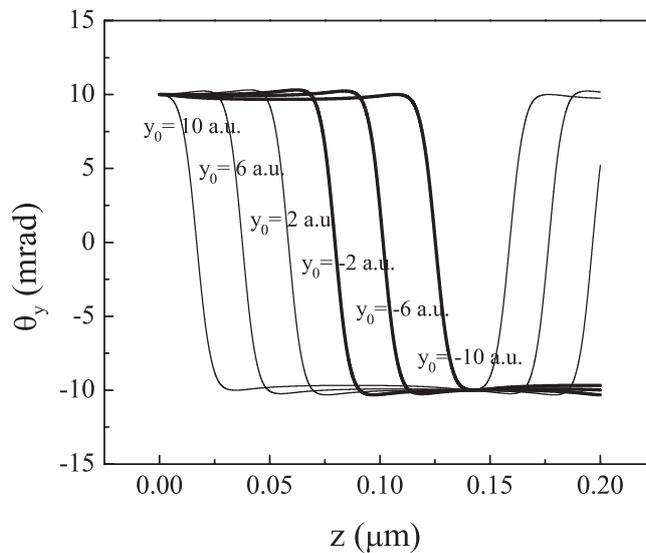
**Figure 12.** The dependence of the  $y$ -component of the proton position on the  $z$ -component of its position in the channeling through the (11, 9) SWCNT with the inclusion of the image force when the proton incident angle  $\varphi = 0$  for the  $x$ -component of the proton impact parameter  $x_0 = 0$  and the  $y$ -component of its impact parameter  $y_0 = \pm 2, \pm 6$  and  $\pm 10$  a.u. The proton velocity is  $v = 3$  a.u., the nanotube radius =  $0.689$  nm and the nanotube length  $L = 0.2$   $\mu\text{m}$ .

the same values of the components of the proton impact parameter as in figure 11. One can see that the channeled protons with  $y_0 = \pm 2$  a.u. give rise to the part of the spatial distribution close to the origin. The channeled protons with  $y_0 = \pm 6$  and  $\pm 10$  a.u. contribute to the peripheral part of the spatial distribution.

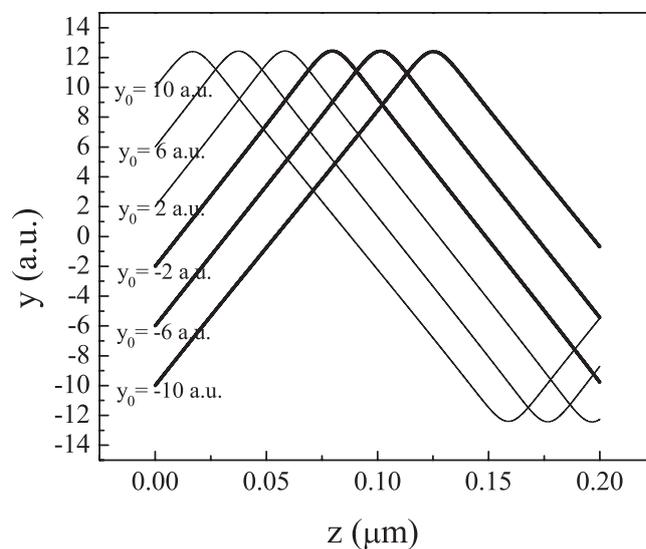
We give in figure 13 the  $y$ -component of the proton scattering angle ( $\Theta_y$ ) as a function of the  $z$ -component of its position with the image force taken into account when  $\varphi = 10$  mrad for the same values of the components of the proton impact parameter as in figure 11. It is easy to conclude that the channeled protons with  $y_0 = 2, 6$  and  $10$  a.u. contribute to the right part of the donut. The channeled protons with  $y_0 = -2, -6$  and  $-10$  a.u. give rise to the most intense part of the donut, being its farthest left part.

Figure 14 shows the dependence of the  $y$ -component of the proton position on the  $z$ -component of its position with the image force included when  $\varphi = 10$  mrad for the same values of the components of the proton impact parameter as in figure 11. It is evident that all the propagating protons in question end up in the left half of the nanotube, after being reflected from the right part of the nanotube wall.

An additional result of our computer simulations is related to the influence of the image force on  $\psi_c$ . We followed the change of the total yield of channeled protons with the increase of  $\varphi$  and found that with the image force taken into account  $\psi_c = 10.6$  mrad. When the image force is not taken into account  $\psi_c = 11.9$  mrad. This increase of  $\psi_c$  is attributed to the increase of the total interaction potential in question, given by equation (2), when its attractive component, originating in the interaction of the proton and its image, is not taken into account. This conclusion is justified via the relation between  $\psi_c$  and the total interaction potential at the



**Figure 13.** The dependence of the  $y$ -component of the proton scattering angle on the  $z$ -component of its position in the channeling through the (11, 9) SWCNT with the inclusion of the image force when the proton incident angle  $\varphi = 10$  mrad for the  $x$ -component of the proton impact parameter  $x_0 = 0$  and the  $y$ -component of its impact parameter  $y_0 = \pm 2, \pm 6$  and  $\pm 10$  a.u. The proton velocity is  $v = 3$  a.u., the nanotube radius  $a = 0.689$  nm and the nanotube length  $L = 0.2 \mu\text{m}$ .



**Figure 14.** The dependence of the  $y$ -component of the proton position on the  $z$ -component of its position in the channeling through the (11, 9) SWCNT with the image force taken into account when the proton incident angle  $\varphi = 10$  mrad for the  $x$ -component of the proton impact parameter  $x_0 = 0$  and the  $y$ -component of its impact parameter  $y_0 = \pm 2, \pm 6$  and  $\pm 10$  a.u. The proton velocity is  $v = 3$  a.u., the nanotube radius  $a = 0.689$  nm and the nanotube length  $L = 0.2 \mu\text{m}$ .

distance from the nanotube wall equal to the screening radius,  $U_{sc}$ ,

$$\psi_c = \sqrt{\frac{U_{sc}}{E}}, \quad (10)$$

where  $E$  is the initial proton energy [49].

#### 4. Concluding remarks

We have presented the first theoretical investigation of the angular and spatial distributions of ions channeled through a nanotube for different proton incidence angles with the effect of dynamic polarization of the nanotube included. The ions are protons with a velocity of  $v = 3$  a.u. and the nanotube is an (11, 9) SWCNT with a length of  $L = 0.2 \mu\text{m}$ . The proton incident angle,  $\varphi$ , is varied between 0 and 10 mrad, being close to the critical angle for channeling,  $\psi_c$ . We have noticed a slight increase of  $\psi_c$  when the image force is not taken into account.

We have observed a ring-like structure developing in the angular distribution of channeled protons with  $\varphi$  increasing and approaching  $\psi_c$ . The effect has been recognized as the donut effect, being in fact the rainbow effect. If  $\varphi$  is between 0 and about  $\psi_c/2$ , the image force plays a significant role in generating the angular and spatial distributions, including the rainbow maxima. However, if  $\varphi$  is close to  $\psi_c$ , the contribution of the image force to the angular and spatial distributions, including the donut effect, is minor.

The analysis of the generated spatial distributions of channeled protons has shown that an increase of  $\varphi$  can give rise to a significant rearrangement of the propagating protons within the nanotube. For example, for  $\varphi = 10$  mrad, the proton beam is displaced from the nanotube axis toward the nanotube wall, leaving the region around the axis practically empty. It is clear that such a rearrangement of the propagating protons may be used to locate various atomic impurities in the nanotube, using the secondary processes like backward Coulomb scattering and nuclear reactions. In addition, the presence of the rainbow maxima in the spatial distributions can be used to determine the positions of the impurities very precisely. One can also think of directing such a nonosized proton beam to a material to be modified with it, or to a biological or medical sample.

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