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Quantum primary rainbows in transmission of positrons through very short carbon nanotubes

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ABSTRACT

This paper is devoted to a quantum mechanical consideration of the transmission of positrons of a kinetic energy of 1 MeV through very short (11, 9) single-wall chiral carbon nanotubes. The nanotube lengths are between 50 and 320 nm. The transmission process is determined by the rainbow effects. The interaction potential of a positron and the nanotube is deduced from the Molire's interaction potential of the positron and a nanotube atom using the continuum approximation. We solve numerically the time-dependent Schrödinger equation, and calculate the spatial and angular distributions of transmitted positrons. The initial positron beam is assumed to be an ensemble of non-interacting Gaussian wave packets. We generate the spatial and angular distributions using the computer simulation method. The examination is focused on the spatial and angular primary rainbows. It begins with an analysis of the corresponding classical rainbows, and continues with a detailed investigation of the amplitudes and phases of the wave functions of transmitted positrons. These analyses enable one to identify the principal and supernumerary primary rainbows appearing in the spatial and angular distributions. They also result in a detailed explanation of the way of their generation, which includes the effects of wrinkling of each wave packet during its deflection from the nanotube wall, and of its concentration just before a virtual barrier lying close to the corresponding classical rainbow. The wrinkling of the wave packets occurs due to their internal focusing. In addition, the wave packets wrinkle in a mutually coordinated way. This explanation may induce new theoretical and experimental investigations of quantum rainbows occurring in various atomic collision processes.

1. Introduction

A positively charged particle is considered as being channeled if it is undergoing a series of correlated small angle collisions with the atoms of the atomic strings defining an axial or planar channel of a crystal [1–3]. The maxima of the yield of particles transmitted through the channel occurring due to the singularities of the mapping of the impact parameter plane to the final transverse position plane or transmission angle plane are called rainbows [4–8]. In accordance with that, the process in which such maxima appear is referred to as rainbow channeling. If the particle kinetic energy is sufficiently high to make the quantum aspects of its behavior negligible, the maxima are called classical rainbows. On the other hand, when the particle kinetic energy is sufficiently low to make the quantum effects dominant, the maxima are designated as quantum rainbows. Each quantum rainbow comprises a principal rainbow and one or more supernumerary rainbows.

Carbon nanotubes are the sheets of carbon atoms lying at the hexagonal crystal lattice sites rolled up into cylinders [9–11]. If the atomic strings of a nanotube spiral around its axis, it is called chiral, and if the atomic strings are parallel to the axis, it is called achiral. Nanotubes can be the single-wall and multi-wall ones, depending on the number of cylinders they contain. The nanotube diameters are of the order of a nanometer and their lengths can be more than a hundred micrometers.

Carbon nanotubes can be used to channel positively charged particles [12]. So far, a number of theoretical groups have studied ion channeling in nanotubes with the main objective to explore the possibility of guiding ion beams with nanotubes [13]. On the other hand, it has been established that rainbows appear in channeling of charged particles in nanotubes as well [14–17]. The experimental studying of ion channeling in nanotubes has not yet been sufficiently developed [18,,19].

Recently, Petrović et al. [17] presented a classical and quantum mechanical investigation of the transmission of positrons through very short (11, 9) single-wall chiral carbon nanotubes. The positron kinetic energies were 1 and 10 MeV while the nanotube lengths

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were 200 and 560 nm, respectively. The analysis was focused on the rainbow effects, which were clearly observed in the spatial and angular distributions of transmitted positrons. The quantum rainbow maxima were explained by the constructive interference of the two rays within the wave packet that started from the points in the impact parameter plane on the two sides of the rainbow point and finished at the same point in the final transverse position plane or transmission angle plane. These authors have used the same approach to explore the possibility of using quantum rainbows for characterization of very short carbon nanotubes [20].

Here, we present a detailed quantum mechanical study of the transmission of positrons of a kinetic energy of $E = 1$ MeV through very short (11, 9) single-wall chiral carbon nanotubes. The nanotube lengths are $L = 50$–320 nm. The corresponding reduced nanotube lengths are $\Lambda = 0.03$–0.19 [5,6,17]. The initial positron beam is taken to be divergent relative to the nanotube axis. Its full-width-at-half-maximum (FWHM) is denoted as Δ_d. The equilibrium nanotube radius is $R_n = 0.69$ nm [10]. The study is a continuation of the studies of Petrović et al. [17] and Ćosić *et al.* [20]. It is focused on the quantum primary rainbows, *i.e.*, the principal and supernumerary primary rainbows, occurring in the spatial and angular distributions of transmitted positrons. We present a detailed analysis of the amplitudes and phases of the wave functions of transmitted positrons, and give a quantum mechanical explanation of the obtained distributions.

2. Theory

The subject of this study is a positron channeled in a nanotube. We choose the z axis to coincide with the nanotube axis; it is the longitudinal axis. The x and y axes are taken to be the vertical and horizontal axes, respectively; they are the transverse axes. The origin lies in the nanotube entrance plane. The nanotube entrance plane is the positron impact parameter plane, the nanotube exit plane is its final transverse position plane, and a plane in between them is a transverse position plane.

2.1. Interaction potentials

In order to describe the interaction of the positron and a nanotube atom, we use the Molière's interaction potential [21]. The needed interaction potential of the positron and nanotube is deduced in three steps. In the first step, we axially average the positron-atom interaction potential, employing the continuum approximation [2]. In the second step, the interaction potential obtained in the first step is azimuthally averaged. This is justified by the facts that the nanotube is chiral and contains even 602 pairs of atomic strings parallel to its axis. The resulting positron-nanotube interaction potential reads

$$U(\rho;R_n) = U_0\sum_{i=1}^{3}\alpha_i K_0\left(\frac{\beta_i R_n}{a_s}\right) I_0\left(\frac{\beta_i \rho}{a_s}\right) \quad \text{for} \quad \rho \leqslant R_n \tag{1}$$

and

$$U(\rho;R_n) = U_0\sum_{i=1}^{3}\alpha_i I_0\left(\frac{\beta_i R_n}{a_s}\right) K_0\left(\frac{\beta_i \rho}{a_s}\right) \quad \text{for} \quad \rho > R_n \tag{2}$$

with

$$U_0 = \frac{16\pi Z_2 e^2 R_n}{3^{3/2} a_b^2}, \tag{3}$$

where $Z_2 = 6$ is the nanotube atom atomic number, e is the elementary charge, $a_s = [9\pi^2/(128Z_2)]^{1/3} a_0$ is the nanotube atom screening radius with $a_0 = 0.026$ nm being the Bohr radius, $a_b = 0.14$ nm is the nanotube atoms bond length [10], $\rho = (x^2 + y^2)^{1/2}$ with x and y being the transverse components of the positron position vector, $(\alpha_i) = (0.35, 0.55, 0.10)$ and $(\beta_i) = (0.1, 1.2, 6.0)$ are the fitting parameters, and I_0 and K_0 denote the modified Bessel functions of the first and second kinds and 0th order, respectively [22]. The Molière's interaction potential with the above given screening radius is chosen because it was employed for a very successful reproduction of a rainbow channeling experiment with an accurate computer simulation code [23]. It is evident that Eqs. (1)–(3) do not contain explicitly the nanotube chiral indices, $m = 11$ and $n = 9$. These indices are hidden in $R_n = [(3^{1/2}/(2\pi)](m^2 + mn + n^2)^{1/2} a_b$ [22].

In the third step, we introduce the thermal vibrations of nanotube atoms [24,17]. This is done in a way appearing as the averaging of the interaction potential obtained in the second step over the effective thermally induced changes of the nanotube radius, R, from its equilibrium value, R_n, along the ρ axis. The positron-nanotube interaction potential is given by

$$U_{th}^{qu}(\rho;R_n) = \frac{1}{(2\pi)^{1/2}\sigma_{th}} \int_{R_1}^{R_2} U(\rho;R) \exp\left[-\frac{(R-R_n)^2}{2\sigma_{th}^2}\right] dR, \tag{4}$$

where $\sigma_{th} = 0.0053$ nm [25] is the one-dimensional thermal vibration amplitude of the nanotube atoms. We take that the integration limits appearing in this expression are $R_1 = R_n - 6\sigma_{th}$ and $R_2 = R_n + 6\sigma_{th}$. They determine the interval in which the changes of the integrand are not negligible. The integration is performed numerically. It should be emphasized that the function $U_{th}^{qu}(\rho;R_n)$ and its first derivative are continuous. However, if one takes into account the fact that the displacements of the nanotube atoms are small, a useful analytical approximation of Eq. (4) can be derived [16,17]. When $\rho \leqslant R_n$, this equation becomes

$$U_{th}^{cl}(\rho;R_n) = U_0\sum_{i=1}^{3}\left(\alpha_i + \frac{\sigma_{th}^2\beta_i^2}{2a_s^2}\right) K_0\left(\frac{\beta_i R_n}{a_s}\right) I_0\left(\frac{\beta_i \rho}{a_s}\right). \tag{5}$$

We have found that this function is continuous and that its deviation from $U_{th}^{qu}(\rho;R_n)$ is very small, especially when $\rho \leqslant R_n - a_s$. However, its first derivative is discontinuous at the point $\rho = R_n$.

In the classical calculations, $\rho \leqslant R_n - a_s$, *i.e.*, the discontinuity of $U_{th}^{cl}(\rho;R_n)$, at point $\rho = R_n$, is not included. Therefore, in this case, we use $U_{th}^{cl}(\rho;R_n)$, given by Eqs. (5) and (3), as the needed positron-nanotube interaction potential. On the other hand, we have found that in the quantum mechanical calculations, the discontinuity of $U_{th}^{cl}(\rho;R_n)$, which cannot be excluded, is a source of serious numerical problems. Consequently, in this case, $U_{th}^{qu}(\rho;R_n)$, given by Eqs. (4) and (1)–(3), is required as the needed interaction potential. It should be noted that $U_{th}^{cl}(\rho;R_n)$ and $U_{th}^{qu}(\rho;R_n)$ are cylindrically symmetric.

We would like to emphasize that $U_{th}^{qu}(\rho;R_n)$ represents a circular potential barrier of a finite height, which means that the positron always tunnels through the nanotube wall, *i.e.*, it is always partly dechanneled. However, it has been found that when the nanotube is very short, the positron dechanneling effect is much less pronounced than the channeling effect.

2.2. Classical approach

The vertical and horizontal components of the initial positron position vector, in the impact parameter plane, are denoted as x_0 and y_0, and the vertical and horizontal components of its initial momentum vector as p_{x0} and p_{y0}, respectively. Further, the vertical and horizontal components of the positron position vector during the channeling are denoted as $x(t)$ and $y(t)$, and the vertical and