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Stationary States of Charged Particles Channeled through Carbon Nanotubes

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Abstract: We investigate the bound states of relativistic positrons channeled in perfect single-walled carbon nanotubes (SWCNTs), with different chiral indices (*n,m*). The channeling potential, has been calculated according to the continuum model approximation given by Lindhard. We find a general expression for the channeling potential fit the calculated channeling potential with fitting parameters for each carbon nanotube. We calculate the energy eigenvalues by, using the WKB method, the energy eigenfunctions and the position probability density of the channeled positron in a plane normal to the nanotube axis by solving the Shrödinger equation using the obtained general formula for the channeling potential.

Keywords: Carbon nanotubes; Relativistic positron beams; Bound states.

1 Introduction

Localization of charged particles in potential wells, regardless of their form, leads to the discretization of the charged particles energy spectrum whereby the distance between energy levels substantially depends on the geometrical size of the potential wells. In the case of channeling of relativistic particles through perfect single-walled carbon nanotubes (SWCNTs), the channeled particles move along the nanotube axis, (*z*-axis) and is influenced by a transverse potential field results from the atomic rows *N*, forming the nanotube surface. The cross section view of perfect nanotube in a plane perpendicular to the tube axis is a circle as illustrated in Fig. 1 for (6,0) nanotube. In previous work [1], the nanotube channeling potential has been calculated for perfect SWCNTs and for radially deformed SWCNTs according to the continuum model approximation given by Lindhard [2] and by using the atomic interaction potential as given by Moliere [3].

In perfect SWCNT, the number of rows *N* for nanotube with chiral indices (*n,m*) is given by, $N = (2/q)(n^2 + nm + m^2)$, where $q = \gcd(2m + n, 2n + m)$ denotes the greatest common divisor of its arguments and the radius of the perfect SWCNT (circular cross section) *R* is given by, $R = (\ell\sqrt{3}/2\pi)\sqrt{n^2 + nm + m^2}$, with $\ell \sim 0.141$ nm, is the bond length between carbon atoms [4].

In this work, we investigate the stationary states of positrons move along the axis of perfect SWCNTs with energy 100 MeV. This study covers the three known types of perfect SWCNTs namely, zigzag, armchair and chiral with different chiral indices (*n,m*). The energy eigenvalues and eigenfunctions and the maximum number of bound states, in a plane perpendicular to the nanotube axis (*xy*-plane), of positrons channeled through perfect SWCNTs have been calculated.

2 Model

We consider the motion of relativistic positrons through SWCNTs in channeling regime, i.e., the channeled positron is assumed to travel as free particle along the nanotube axis, (*z*-axis) and is influenced by the interaction of positron and a nanotube atoms namely, channeling potential in a plane perpendicular to the tube axis (*xy*-plane). The channeling potential

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has been calculated for perfect SWCNTs according to the continuum model approximation. According to this approximation, the interaction between positrons and one row of the nanotube is given by

$$U(r)=\frac{2\,z_1z_2e^2}{d_R}\sum_{i=1}^{3}\alpha_iK_0(\beta_ir), \tag{1}$$

with $\{\alpha_i\}=\{0.35,0.55,0.1\},\{\beta_i\}=\{0.3/a,1.2/a,6/a\}$ where $a=(9\pi^2/128\,z_2)^{1/3}a_0$, is the Thomas-Fermi screening radius; $a_0=0.529\,\text{Å}$ is the Bohr radius, z_1 and z_2 are the charge numbers of channeled particle and nanotube atoms respectively, r is the separation between the row and the channeled particle in a plane perpendicular to the nanotube axis, d_R is the average distance of neighboring carbon atoms along the row ($d_R=(3\ell/q)(n^2+nm+m^2)^{1/2}$ [4]), e is the elementary charge and K_0 is the modified Bessel function of the second kind and order zero.

Now, by using Eq. (1), the channeling potential, $U(\rho)$, due to all rows of the SWCNT is the sum of the axial continuum potentials of all rows positioned over the circumference of the nanotube, where ρ is a vector measured from the nanotube center (Fig. 1), is given by

$$U(\rho)=\sum_{j=1}^{N}U(|R_j-\rho|), \tag{2}$$

where R_j, is the distance of row number j from the nanotube center. In the numerical calculation of Eq. (2), we note that, the N atomic rows consists of two sequences of rows overlap i.e., with a doubled linear atomic density, $2/d_R$.

The effect of thermal vibrations on channeling potential in carbon nanotube can be estimated by modification in the axial potential. The axial potential at large distance from the nanotube wall due to one raw modified by the effect of thermal vibration is given by [5]:

$$U_{th}(r)=\frac{2z_1z_2e^2}{d_R}\sum_{i=1}^{3}\alpha_iK_0(\beta_ir)e^{(u^2/2\alpha_i^2)}, \tag{3}$$

where u is the thermal vibrational amplitude of the carbon atoms estimated from the Debye approximation [6]. The numerical results showed that the effect of thermal vibrational amplitude on the channeling potential, at temperature ~ 790 K (i.e., at thermal vibrational amplitude $u\approx 0.0053\ nm$), is very small and gave approximately the same results as that for the channeling potential of static nanotube at nanotube axis [7,8] .

In perfect SWCNT, all atomic rows are positioned at equal distance $R_j=R$ from the nanotube center O and distributed on the circumference at equal distances, $2\pi R/N$, thus we have N lines connecting the atomic rows and the nanotube center in the xy- plane. In this representation we consider the line number one (i.e., $j=1$) as the reference line. As illustrated in Fig. 1, the line number j makes an angle

$$\theta_j=2\pi(j-1)/N, \tag{4}$$

with the reference line. Thus, the reference line makes an angle $\theta_1=0$, i.e., directed along the x-axis in the xy-plane, and the line with $j=2$ makes an angle $\theta_2=2\pi/N$ and so on for all lines where $j=1\to N$. Now it is obvious that any two successive lines, R_j and R_{j+1}, subtend a central angle, $2\pi/N$.

Now, by using Eqs. (1)-(4), the channeling potential at any point at a distance ρ from the center of the nanotube could be calculated from the following expression:

$$U(\rho)=\frac{4z_1z_2e^2}{d_j}\sum_{j=1}^{N}\sum_{i=1}^{3}\alpha_iK_0(\beta_i(\rho^2+R^2-2\rho R\cos\theta_j)^{1/2})e^{(u^2/2\alpha_i^2)} \tag{5}$$

For all nanotubes under consideration, we find an expression of the form

$$U(\rho)=a+be^{c\rho} \tag{6}$$

is a good approximation for the channeling potential in perfect SWCNTs calculated according to the continuum model approximation for nanotubes with various chiral indices (n,m). The parameters a,b and c fit the calculated channeling potential are given in Table 1. Now, the bound states of the channeled positron could be calculated by solving the Shrödinger equation of motion in the transverse direction to the nanotube axis using the potential function (6) as follows

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{d\rho^2}+[(a+be^{c\rho})-E]\ \psi(\rho)=0 \tag{7}$$

Table 1. Values of the parameters a, b and c in Eq. (7) needed to fit the nanotube channeling potential for the given (n,m) nanotubes, n_{max} is the maximum number of bound states for channeled positron.

(n,m)	Radius (nm)	a (eV)	b (eV)	c (nm^{-1})	n_{max}
(6,0)	0.23321	14.56240	1.71635	15.62744	13
(8,0)	0.31095	7.39359	0.44004	16.61130	14
(5,5)	0.33661	4.88444	0.99497	12.62148	18
(8,8)	0.53858	0.64276	0.09489	12.32286	19
(8,2)	0.35624	4.11171	0.71212	12.96176	18
(11,5)	0.55106	0.57011	0.07542	12.53133	19

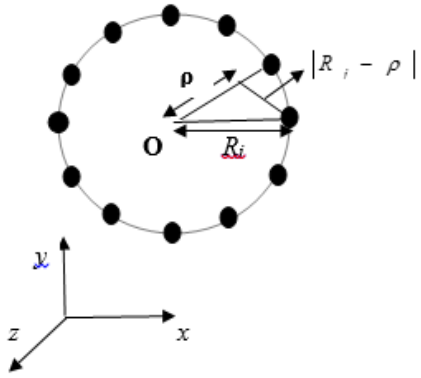

Figure 1. Cross section view of (6,0) perfect nanotube, the cross section of the nanotube channel is a circle of radius R, the rows of the carbon atoms are positioned at R_j over the circumference of the nanotube, ρ the distance from the nanotube center in a plane perpendicular to the tube axis.

3 Eigenfunctions of the Channeled Positrons

The wave function of the channeled positron in the transverse plane to the nanotube axis is obtained via positron Shrödinger equation given by Eq. (7). The change of variables $y=\left(\frac{8mb}{\hbar^2c^2}\right)^{1/2}e^{c\rho/2}$ transforms this eigenvalue equation (7) into

$$y^2\frac{d^2\psi(y)}{dy^2}+y\frac{d\psi(y)}{dy}-\left(y^2+\nu^2\right)\psi(y)=0 \tag{8}$$

where $\nu=i\sqrt{\frac{8m}{\hbar^2c^2}(E-a)}$. This is Bessel's equation in modified form with index ν [9]. This second order differential equation has two linearly independent solutions, the modified Bessel functions of the first and second kind, $I_\nu(y)$ and $K_\nu(y)$, so the general solution of equation (8) may be written as follows

$$\psi(y)=c_1I_\nu(y)+c_2K_\nu(y)$$

We then need to impose the boundary condition $\psi\big|_{y\to\infty}=0$. By definition, $I_\nu(y)$ is exponentially increasing, then condition at infinity requires that we set the coefficient of $I_\nu(y)$ to zero. The condition at $\rho=0$ then simply requires that $K_{i\sqrt{8m(E_n-a)/\hbar^2c^2}}\left(\left(\frac{8mb}{\hbar^2c^2}\right)^{1/2}\right)=0$. The eigenfunctions are of the form

$$\psi_n(\rho)=C_nK_{i\sqrt{8m(E_n-a)/\hbar^2c^2}}\left(\left(\frac{8mb}{\hbar^2c^2}\right)^{1/2}e^{c\rho/2}\right) \tag{9}$$

4 Eigenvalues of the Channeled Positrons

The energy eigenvalues of the channeled positrons constrained to move between classical turning points $-\rho$ and ρ in a potential as given by Eq. (6) have been calculated by using the WKB method [10]. The classical turning points are those points at which $U(\rho)=E$ that is: $E=a+be^{c\rho}$

or

$$\rho=\frac{1}{c}\ln\frac{(E-a)}{b} \tag{10}$$

For a particle constrained to move between classical turning points $-\rho$ and ρ in a potential well, the energy eigenvalues can be obtained from the condition:

$$\int_{-\rho}^{\rho}pd\rho=(n+\frac{1}{2})\pi\hbar\,,\qquad n=0,1,2,..... \tag{11}$$

where $p=\left[2m\left(E-\left(a+be^{c\rho}\right)\right)\right]^{1/2}$, is the classical linear momentum. Then, from Eqs. (10) and (11), we can get the energy eigenvalues and the maximum number of bound states respectively as:

$$E_n=a+\left(\frac{1}{2m}\right)\left(\frac{c\pi\hbar}{2\ln 2}\right)^2(n+\frac{1}{2})^2 \tag{12}$$

and

$$n_{\max}=\left(\frac{2\ln 2}{c\pi\hbar}\right)\left[2m(E_{\max}-a)\right]^{1/2}-0.5 \tag{13}$$

where E_{max}, is the potential at the turning points, that is, $E_{\max}=a+be^{cs}$, $s=R-a$, is the screening length,

5 Computational Results and Discussion

The channeling potential has been calculated for perfect SWCNTs. The calculations covered (6,0), (8,0), (5,5), (8,8), (8,2) and (11,5) tubes at nanotube temperature ~ 790 K, (i. e, at thermal vibration amplitude u_1 = 0.0053 nm), by using Debye approximation as a function of a distance ρ from the center of the tube in a plane normal to the tube axis is shown in Fig. 2. The numerical results showed that the effect of temperature on the channeling potential is very small and gave approximately the same results as that for the static nanotube at nanotube center.

The energy eigenfunctions and the position probability density in the transverse plane to the nanotube axis for the first three states of positrons channeled in perfect SWCNTs with incident energy 100 MeV in a direction parallel to the nanotube axis is illustrated in Figs. 3, 4, 5, 6, 7, and 8, respectively. The position probability density has its maximum value at nanotube center ($\rho=0$) and decreases as ρ increases (i.e., towards the nanotube wall).

The energy eigenvalues of the channeled positrons as calculated from Eq. (12) in different types of single-walled carbon nanotubes are given in Table 2. The maximum number of bound states, as calculated from Eq. (13), are given in Table 1. The calculations show that the estimated maximum number of bound states increases as the nanotube radius increase for zigzag, chiral and armchair carbon nanotubes.

Table 2. Energy eigenvalues of positrons with incident energy 100 MeV in a direction parallel to the nanotube axis channeled in different types of single-walled carbon nanotubes calculated by using WKB approximation.

Bound state	Zigzag (*n*,0)		Armchair (*n*,*n*)		Chiral (*n*,*m*)	
E_n	(6,0)	(8,0)	(5,5)	(8,8)	(8,2)	(11,5)
E_0	14.6231	7.4622	4.9240	0.6805	4.1535	0.6092
E_1	15.1089	8.0110	5.2409	0.9825	4.4876	0.9215
E_2	16.0803	9.1087	5.8746	1.5866	5.1560	1.5461
E_3	17.5375	10.7551	6.8251	2.4927	6.1584	2.4832
E_4	19.4805	12.9504	8.0925	3.7008	7.4951	3.7325
E_5	21.9091	15.6945	9.6767	5.2109	9.1658	5.2941
E_6	24.8235	18.9874	11.5777	7.0231	11.1708	7.1681
E_7	28.2237	22.8292	13.7956	9.1373	13.5099	9.3544
E_8	32.1095	27.2197	16.3303	11.5535	16.1831	11.8531
E_9	36.4811	32.1591	19.1819	14.2718	19.1905	14.6641
E_{10}	41.3385	37.6473	22.3503	17.2919	22.5321	17.7874
E_{11}	46.6816	43.6843	25.8356	20.6143	26.2078	21.2231
E_{12}	52.5104	50.2702	29.6377	24.2387	30.2177	24.9711
E_{13}		57.4048	33.7567	28.1649	34.5618	29.0314
E_{14}			38.1925	32.3934	39.2400	33.4041
E_{15}			42.9451	36.9238	44.2523	38.0890
E_{16}			48.0146	41.7562	49.5988	43.0863
E_{17}			53.4009	46.8907	55.2795	48.3961
E_{18}				52.3272		54.0180

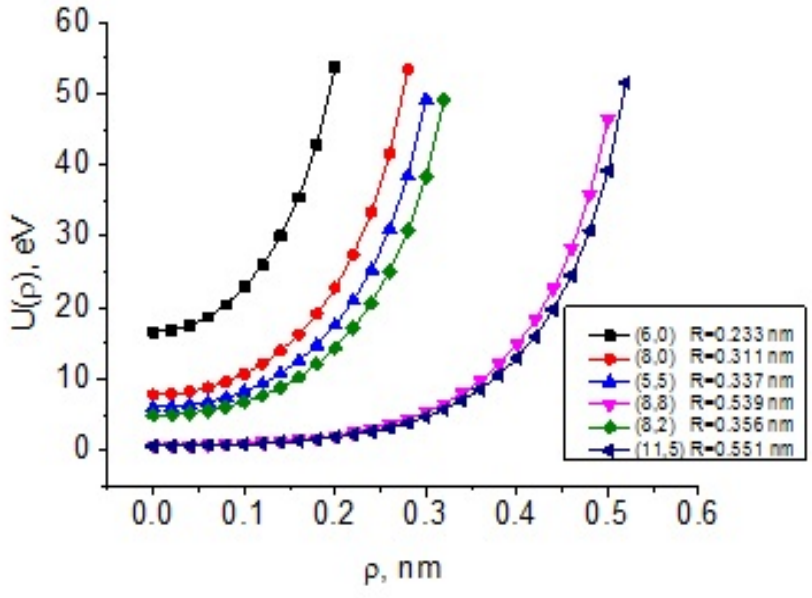

Figure 2. Channeling potential for positrons channeled in single-walled Carbon nanotubes with different chiral indices (*n*,*m*) as a function of the distance ρ from the nanotube center in a plane normal to the nanotube axis.

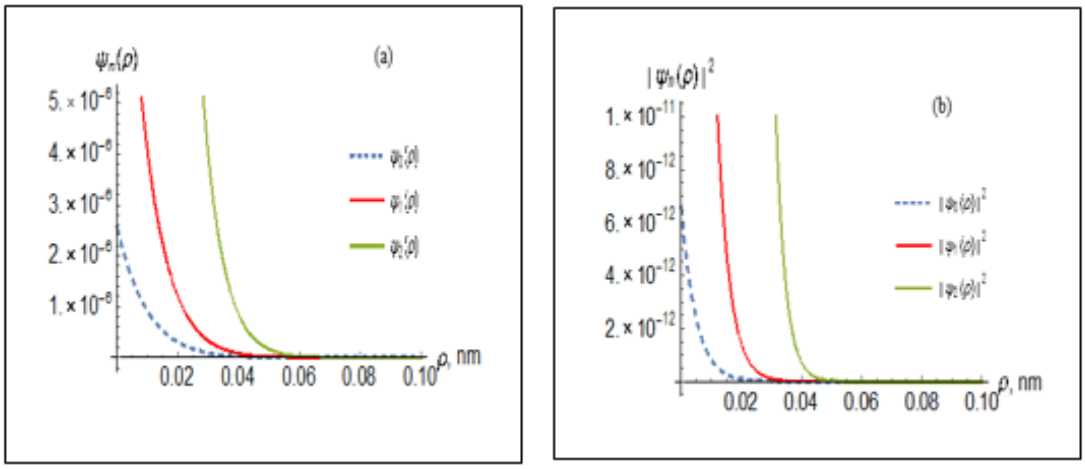

Figure 3. The first three states of positrons channeled in single-walled carbon nanotube (6,0) with incident energy 100 MeV in a direction parallel to the nanotube axis. (a) Energy eigenfunctions, (b) The position probability density.

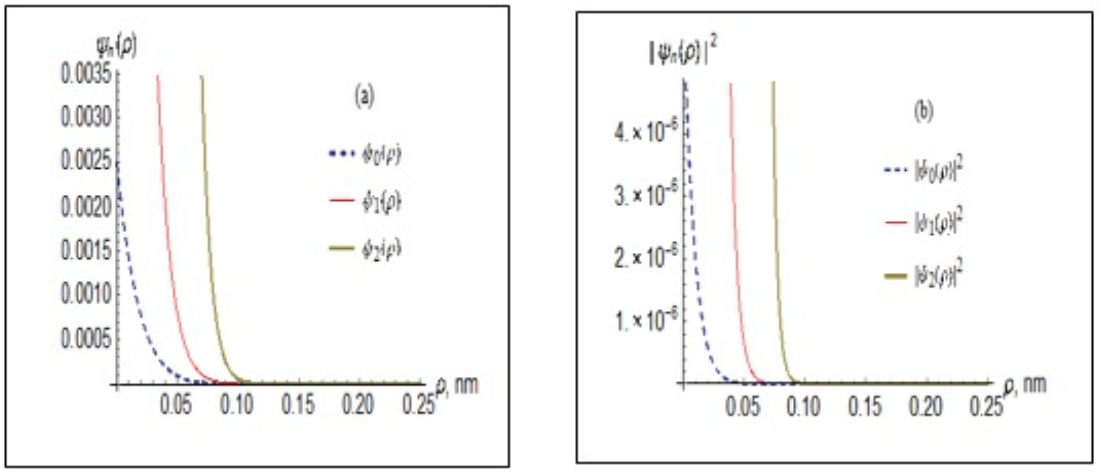

Figure 4. The first three states of positrons channeled in single-walled carbon nanotube (8,0) with incident energy 100 MeV in a direction parallel to the nanotube axis. (a) Energy eigenfunctions, (b) The position probability density.

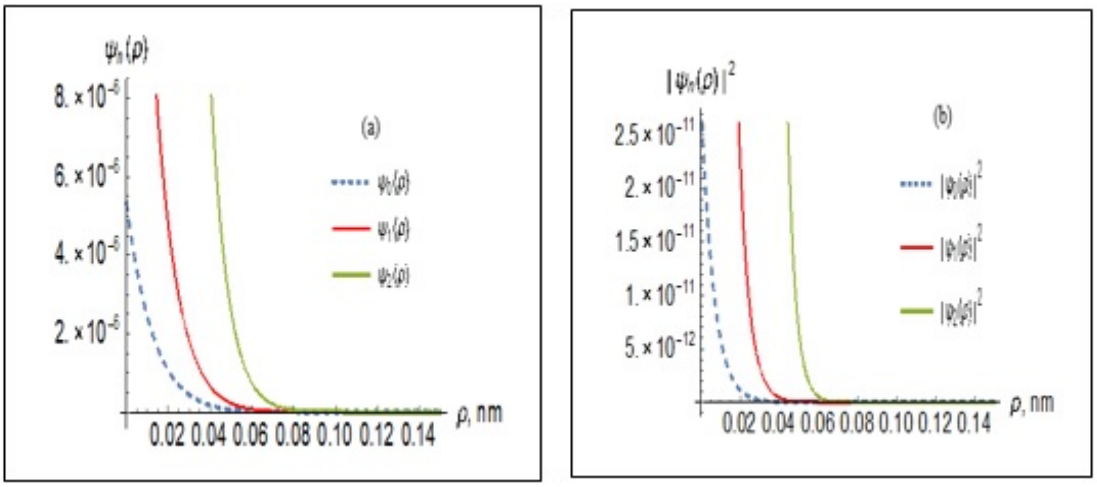

Figure 5. The first three states of positrons channeled in single-walled carbon nanotube (5,5) with incident energy 100 MeV in a direction parallel to the nanotube axis. (a) Energy eigenfunctions, (b) The position probability density.

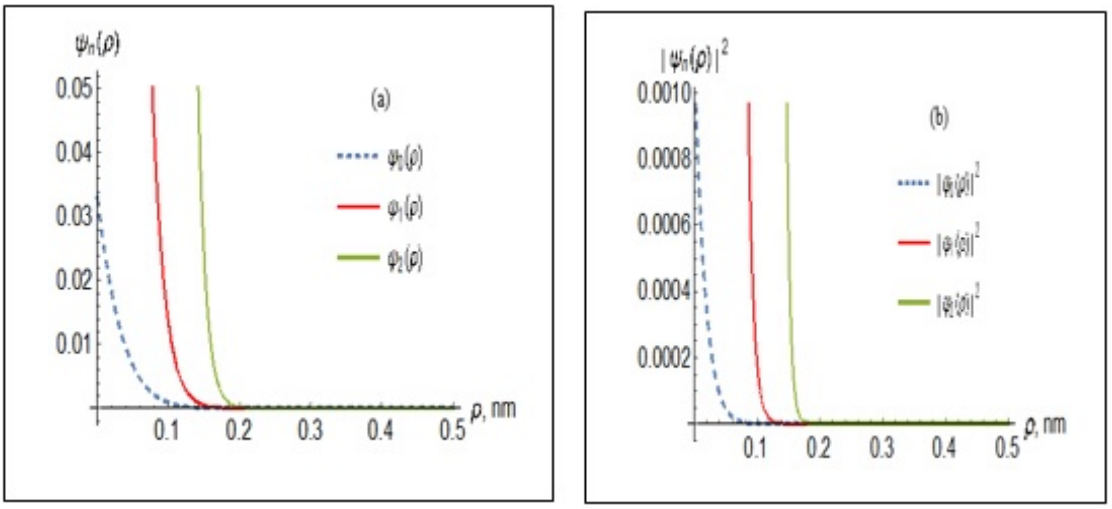

Figure 6. The first three states of positrons channeled in single-walled carbon nanotube (8,8) with incident energy 100 MeV in a direction parallel to the nanotube axis. (a) Energy eigenfunctions, (b) The position probability density.

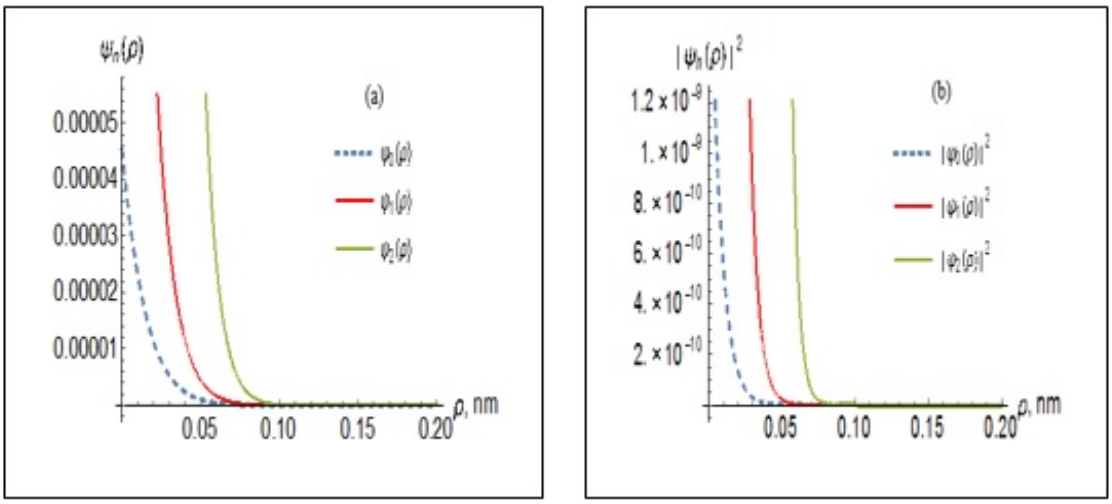

Figure 7. The first three states of positrons channeled in single-walled carbon nanotube (8,2) with incident energy 100 MeV in a direction parallel to the nanotube axis. (a) Energy eigenfunctions, (b) The position probability density.

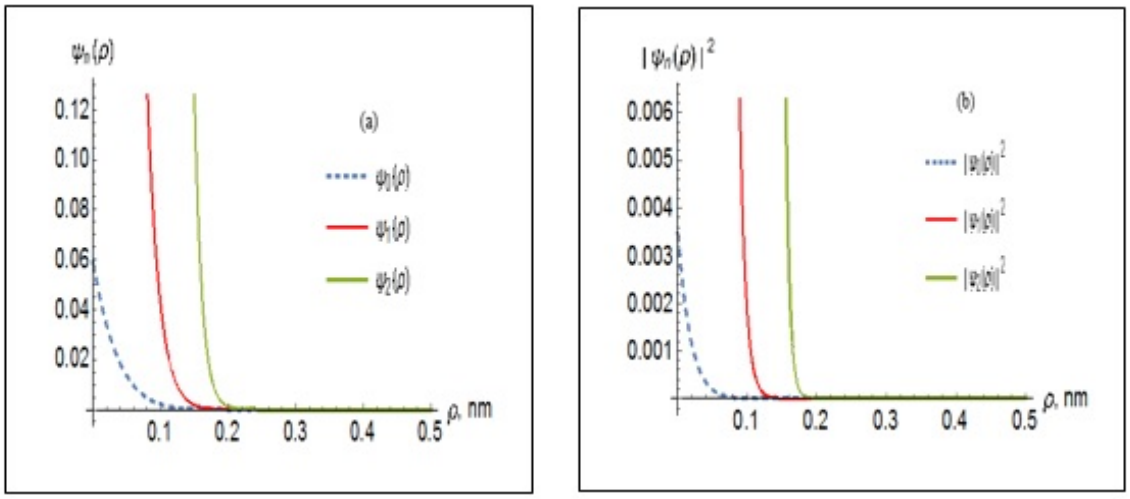

Figure 8. The first three states of positrons channeled in single-walled carbon nanotube (11,5) with incident energy 100 MeV in a direction parallel to the nanotube axis. (a) Energy eigenfunctions, (b) The position probability density.

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