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**COMMUNICATION**

# Resonance Transitions in the Cylindrical Barrier as Related Carbon Nanotube States

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## ABSTRACT

The solution of the Schrödinger equation in a cylindrical coordinate system is considered. The carbon nanotube is modeled by a cylindrical tunnel barrier with periodic boundary conditions. An expression is obtained for the charge current depending on the radius and length of the nanotube. Shown that the current vector has a radial component that changes the sign for certain transitions with large index values. The occurrence of negative values of the current component indicates the presence of negative differential conductivity for these transitions. The appearance of additional current peaks serves as an indication of the excitation of the tunnel system by the external field. This makes it possible to further tune into resonance, which can be carried out by adjusting the "longitudinal" component of the current, depending on the length of the nanotube.

***Keywords:*** Carbon Nanotube; Potential Barrier; Cylindrical Coordinates; Energy States; Current

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# 1. Introduction

Currently, elements are used to detect weak electromagnetic radiation flows, the principle of which is based on excitation of quantum states in structural components of materials. At the same time, macroscopic properties of materials that change their parameters under the influence of an external field are used to detect electromagnetic fields of the radio frequency range. Weak field detection requires a signal amplification system, which is often a complex system of semiconductor elements with a large noise level. In this regard, of particular interest is the regular structure of resonance-tunnel diodes, which allows, due to resonance transfer, to sharply strengthen the signal without distorting the form. The main way to solve the problem is to create a multi-barrier nanostructured material operating on the principle of resonant charge transfer and having external control of the electromagnetic field.

The use of carbon nanotubes for the purpose of generating/receiving terahertz electromagnetic radiation attracts increasing attention due to the high degree of miniaturization and the possibility of creating highly sensitive receiving devices [1–6]. Resonance tunneling and the effect of negative differential conductivity in nanostructures are caused by purely quantum phenomena of spatial quantization, leading to the emergence of resonant energy levels. Such effects allow the development of new properties of nanomaterials [2,3].

# 2. Theoretical Background

The use of carbon nanotubes (CNT) seems promising for the purposes of detecting variable fields in the terahertz range due to spectral features of CNT [7,8]. This is due to the fact that single-layer CNTs have a different kind of spectrum depending on the chirality of the tube. The chirality of CNT determines the symmetry of the arrangement of carbon atoms and the structure of CNT.

The chirality indices of the single layer nanotube (m, n) unambiguously determine its diameter D:

$$D = \sqrt{3\left(m^2 + n^2 + nm\right)}\ d_0 / \pi \tag{1}$$

where $d_0$ = 0.142 nm is the distance between adjacent carbon atoms in the graphite plane.

For different CNT, the area structure of the spectrum has a different appearance [1] (**Figure 1**):

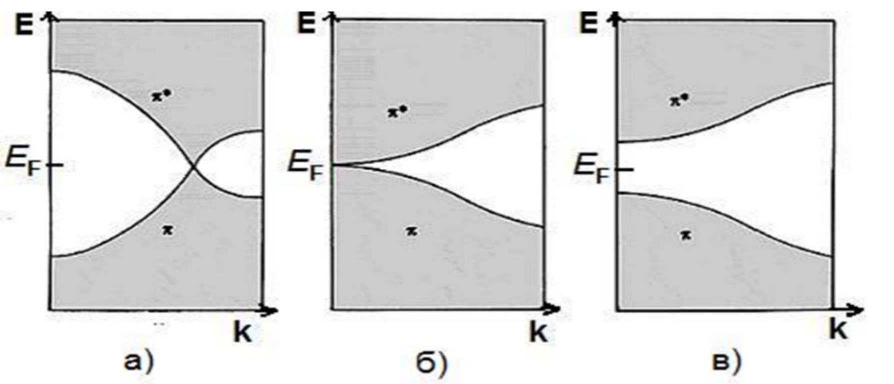


**Figure 1.** Nanotube zone structure depending on chirality index. **a**) metal tubes (n, *n*b) metal tubes (*n,* 0), if n is a multiple of 3. **c**) semiconductor tubes (*n,* 0), n is not a multiple of 3.

For such spectrum species, it has been shown [9–12] that CNTs have their own characteristics in quantum properties.

It should be noted that the resonance frequency thus calculated has a fairly conditional character, since it does not take into account other processes that occur when absorbing an external electromagnetic field. For example, if there are several CNTs located at a certain distance from each other, it is necessary to take into account the linear inductance and the capacity of two or more conductors in the line. Considering two CNTs, as a model of a receiving antenna (**Figure 2**), it is necessary to take into account the mutual capacity, which is determined by the ratio of the length of the CNTs to their diameter. Therefore, in the receiver all this makes the above estimate of the resonant frequency made in order of magnitude.

In addition, the proposed mechanism for delaying the movement of charge carriers does not provide a clear justification for such inductance and capacitance values that are proportional to the Fermi velocity. The above expressions suggest a complex structure of the Fermi level in the CNT. The explanation of the mechanism may become more transparent, given that the CNT is a cylindrical barrier with a non-trivial state structure. Moreover, these states are located near the carbon cells that make up the base of the CNT.

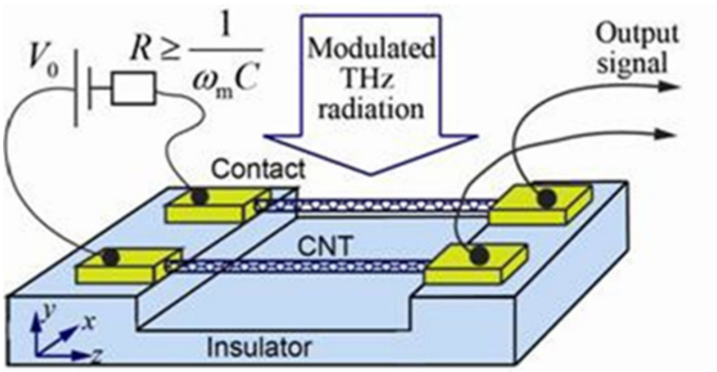


**Figure 2.** Model of receiving antenna on two nanotubes [2].

# 3. Mathematical Modelling

To find a spectrum within a potential barrier, it is necessary to solve the Schrödinger equation in a cylindrical coordinate system. Here, it should be noted that when considering tunneling processes, a one-dimensional problem [13] is usually solved, as a rule, in a Cartesian coordinate system. However, as will be shown below, the solution in the cylindrical coordinate system has a richer spectrum of states. We also note that the solution of the Schrödinger equation in a cylindrical coordinate system has been known for a long time [14,15], and in its most general form. For the purposes of analyzing resonance tunneling conditions, the solution of the first boundary problem in the variable separation method is summarized.

Let's write the Schrödinger equation in a cylindrical coordinate system:

$$-\frac{\hbar^2}{2M}\left[\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial\psi}{\partial r}+\frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2}+\frac{\partial^2\psi}{\partial z^2}\right]+U_0\psi=E\psi \quad (2)$$

Here, the condition ($U_0$ is the height of the barrier) is imposed on the value of the potential:

$$\boldsymbol{U}=\begin{cases}U_0 & 0\le r\le R;\,0\le z\le L\\ 0 & r>R,\,z>L\end{cases} \quad (3)$$

Solution of the first boundary problem, in the method of variable separation, we write in the form:

$$\psi(r,\phi,z)=CJ_n(kr)e^{i(s\phi+jz)} \quad (4)$$

Where $k^2 = [2M(-U_0/h^2]$, $Jn(x)$– the Bessel function of the integer index, s, j are integers. Spectrum of states within the barrier:

$$E_{ik}=U_0-\frac{\hbar^2}{2M}\left(\frac{\mu_i^2}{R^2}\right) \quad (5)$$

Where are the real $\mu_i$ roots of the equation $Jn(\mu_i R) = 0$, n = 0.1,2,3....... To determine the normalization constant, use the conditional orthogonality of the Bessel functions.

$$\int_0^1 J_m(\mu_i x)J_m(\mu_k x)x\,dx=\begin{Bmatrix}0, & i\neq k\\ \frac{1}{2}[J_{m+1}(\mu_i)]^2, & i=k\end{Bmatrix} \quad (6)$$

After simple transformations, we get: $C = \sqrt{2} / J_{m+1}(\mu_i R)$. Note that the normalization constant is determined by the roots of the Bessel function of m + 1st order. In addition, it depends on the roots of the Bessel function at the border of the cylindrical barrier.

This expression for the spectrum of states is due to the selected variable separation method. In the z direction, wave functions have the form of sines or cosines, and in the plane r and β are determined by Bessel functions, which include s and j, which play the role of "magnetic" quantum numbers.

Some values of the roots of the equation $J_n(kR) = 0$ are presented in **Table 1**.

The type of wave functions, depending on the argument and index (s, j = 0) is shown in **Figure 3**.

**Table 1.** The first five roots of the Bessel functions of the whole index.

| $Root_s$ | J0(x) = 0 | J1(x) = 0 | J2(x) = 0 | J3(x) = 0 |
|---|---|---|---|---|
| 1 | 2.405 | 3.832 | 5.136 | 6.380 |
| 2 | 5.520 | 7.016 | 8.417 | 9.761 |
| 3 | 8.654 | 10.173 | 11.620 | 13.015 |
| 4 | 11.791 | 13.324 | 14.796 | 16.223 |
| 5 | 14.931 | 16.471 | 17.960 | 19.409 |

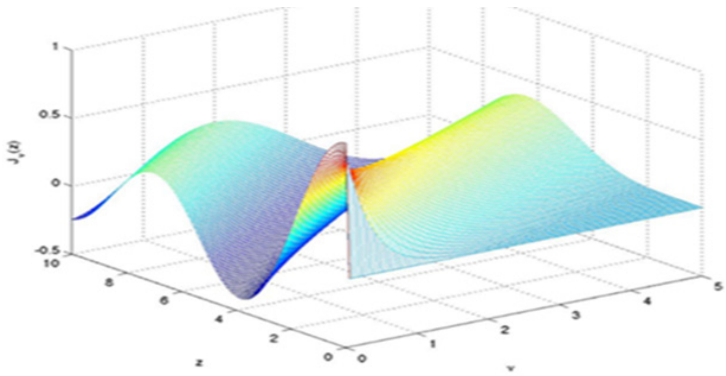


**Figure 3.** The appearance of the Bessel function depends on the argument and index.

## 4. Results and Discussion

Consider the amount of current caused by the motion of the charges. Using the standard expression for current [14]:

$$I_{mn}^{a} = iC^2\left(\psi_m^*\nabla\psi_n - \psi_n\nabla\psi^*{}_m\right) \quad (7)$$

performing simple but cumbersome transformations using the gradient representation in cylindrical coordinates and the relationship between Bessel functions,

$$\frac{d\,J_n(\rho)}{d\rho} = \left\{\frac{1}{2}J_{n-1}(\rho) - J_{n+1} + (\rho)\right\} \quad (8)$$

get expressions for components of the current vector in state n:

$$I_\rho = 0\,; \quad (9)$$

$$I_\varphi = e\frac{\hbar}{\mu}C_1^2[\frac{s}{r}J_n(\rho)J_n(\rho)] \quad (10)$$

$$I_z = e\frac{\hbar}{\mu}C_1^2 j[J_n(\rho)J_n(\rho)] \quad (11)$$

where $\rho = kr$, $C_1 = [J_{n+1}(kR)J_{n+1}(kR)]^{-1}$

Based on the type of wave functions, it should be noted that several additional terms appear in the expression for current through the barrier. Taking into account the harmonic dependence of wave functions on ϕ and z, additional local maxima appear that confirm significant probabilities of transitions through states with large order values. Taking into account the close values ϕ find z of the roots of the Bessel functions of large orders, there is the possibility of transitions between states with energies of the terahertz range. By changing the size of the barrier due to the application of an external electric field, it becomes possible to control the spectrum of states and more precisely adjust to resonant transitions.

A feature of the structure of expressions for current in states (8–10) is the dependence on the radial coordinate, although the radial component is zero. This results in a spiral view of the current density (**Figure 4**).

Accordingly, the magnitude of the magnetic moment will be similar. All this leads to a non-trivial dependence of the current on the applied external magnetic field.

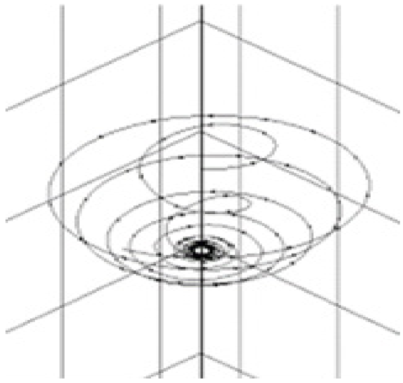

**Figure 4.** Helical movement of charges in the cylindrical barrier. ( n = s = j =1).

Calculating the current between n ≠ m states leads to the appearance of a radial component, moreover, imaginary. It means that the radial component is responsible for absorption of the external field on transitions with different n ≠ m.

$$I_\rho = -ie\frac{\hbar}{\mu}C_2{}^2\{ J_n(\rho)\,[\,J_{m-1}(\rho) - J_{m+1}(\rho)\,] - J_m(\rho)\,[\,J_{n-1}(\rho) - J_{n+1}(\rho)\,]\,\} \quad (12)$$

$$I_\varphi = e\frac{\hbar}{\mu}C_2{}^2[\frac{s}{\rho}J_n(\rho)J_m(\rho)] \quad (13)$$

$$I_z = e\frac{\hbar}{\mu}C_2{}^2\, j[J_n(\rho)J_m(\rho)] \quad (14)$$

here - $C_2 = [J_{n+1}(kR)J_{m+1}(kR)]^{-1}$ It should be noted that the radial component of the current enters only the reactive part, and the angular and longitudinal component enters the active part.

Integrating by ρ we get for intra-zone current (9–11) different from zero angular and longitudinal components, which are quantized by numbers s and j. For the current between different states (inter-zone current (12–14)) after integration with ρ, only the radial term remains, which changes the sign at large indices (n,m > 2)

A characteristic feature of the radial component of the “interzonal” current is the change in its sign for certain ratios n ≠ m. This results in negative differential conductivity, which provides signal amplification. Thus, the assumption of resonant signal amplification at certain transitions between n ≠ m. By summing by n, m, we obtain that the radial component of the interzonal current is zero. This confirms absorption gain compensation at various transitions within the barrier. At the same time, the angular and longitudinal components coincide with the accuracy of a constant numerical factor.

In addition, current movements through states with large values of n and m, due to the interleavability property of the roots of the equation $J_n(kR) = 0$ it possible to control frequency dependence of current on external field. Indeed, the difference in E values for n,m the various n and implicitly, through the dependence of the roots on the height of the potential barrier, is determined by the value of the applied field. This makes it possible to further tune into resonance, which can be carried out by adjusting the “longitudinal” component of the current, depending on the length of the nanotube.

If you determine the frequency for the difference in states with large indices, then due to the interleavability of the roots of Bessel functions, you can find states with frequencies of the order of several terahertz. This fact allows us to suggest that the states of the CNT, as a cylindrical barrier are determined by the quantum inductance and capacitance of the CNT.

## 5. Conclusions

The proposed interpretation of the appearance of quantum inductance and CNT, capacitance is qualitative. On the other hand, it allows you to express considerations about the physical mechanism of the appearance of such properties of CNTs.

The appearance of additional current peaks serves as an indication of the excitation of the tunnel system by the external field. Therefore, by changing the value of the field, it is possible to resonantly adjust the system of nanotubes to a certain frequency of the external field[16,17].

Such a system is purely electric and allows a wide range of potential values for tuning to resonance with an external field.

This is all the more necessary because such a system of nanotubes has a high sensitivity of resonant tunneling to the magnitude of the external field. The creation of a regular grille from RTD will allow the development of devices that display incident electromagnetic waves with a frequency of up to tens of terahertz. Such grilles can be widely used not only in receiving devices, but also for sensitive sensors for medical purposes.

At the same time, the reverse process, the quasi-resonant absorption of the external field in such a structure, is of considerable interest. Such absorption leads to a change in the conditions for the passage of the barrier and, accordingly, a change in the value of the current and electric field [18].

In a real situation, there is a need to take into account the influence of the always present interaction between electrons on the processes of quantum interference and resonance tunneling. The latter follows from the fact that the shift of the resonant level due to interaction is small compared to the energy of the electron, but comparable to the width of the resonant level, dramatically changing the resonant current. This shift can be due to the application of an external field, and a low frequency.

The creation of a regular grille from RTD will allow the development of devices that display incident electromagnetic waves with a frequency of up to tens of terahertz. Such grilles can be widely used not only in receiving devices, but also for sensitive sensors for medical purposes.

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"Not applicable." for studies not involving humans or animals.

## Informed Consent Statement

"Not applicable." for studies not involving humans.

## Data Availability Statement

All data generated or analyzed during this study are included in this article.

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## Conflicts of Interest

The authors declare no conflict of interest.

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