OPTICAL CONDUCTIVITY OF METALLIC NANOTUBES

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Explicit expression for optical conductivity of a metallic nanotube as a function of its inner and outer radii and the ratio between the photon energy and the Fermi energy is obtained. A correction to the expression of optical conductivity caused by quantization of electrons' energy inside a metallic nanotube is obtained in an explicit form; the oscillation of the correction as a function of the light frequency is established.

Introduction

In recent years, physics of small clusters has been separated as a promising direction of physical science. As is known, small clusters of a substance possess properties essentially different from those of a bulk substance. For example, island films emit electrons and photons under a relatively low pumping power [1] (bulk metals do not exhibit such effects under the same level of power).

A distinct place among the fine clusters occupy structures of about 1-nm size, but only in two dimensions — the thin metallic wires (see, for instance, [2]), whose optical properties were theoretically investigated in [3].

If one considers the thin metallic wires, quantization of the electron spectrum becomes topical. The electron spectrum discreteness can manifest itself in a variety of effects.

In [4], the manifestation of the electron energy quantization in thin metallic wires is investigated experimentally in the phenomena of electroluminescence and conductivity. In that work, hot electrons generated due to a potential difference caused the light emission applied. Theoretical study of quantization effects in such cylindrical metallic conductors is done in [3, 5]. In particular, it was shown in [5] that oscillations can occur on the graph of conductivity as a function of the frequency of the current-inducing electric field.

In works [3, 5], the asymptotic form of radial electron functions was used to find the electron spectrum. Such an approach put certain limitations on the radius of the cylindrical conductor and did not allow a wide-range changing of a gap between the electron energy levels. Consideration of the metallic nanotubes undertaken in this work is free of such limitations. In the case of the nanotubes, one can change the tube's inner radius and thickness of the cylindrical cover independently of each other, so the interlevel gap can be varied in a wide range within the limits of applicability of the asymptotics of the electron wave functions.

A technology of fabrication of metallic nanotubes is described, for example, in [6, 7].

This work is devoted to study of optical (high-frequency) conductivity and its oscillations caused by the electron spectrum quantization in thin-wall metallic nanotubes.

1. Setting of the Problem. Electron Wave Functions

Let us consider a metallic nanotube (hereinafter metallic nanotube is considered as a cylindrical metallic envelope only, without the carbon nanotube) as a potential axisymmetric well for electrons; here we introduce the cylindrical coordinate system. The electron potential depends on the radial variable, as shown in Fig. 1.

Let an electromagnetic wave be incident perpendicularly to a tube represented by such a model potential. (The perpendicular incidence is presumed to avoid the Drude absorption connected with movement of electrons along a nanotube.) We consider a light absorption in such a tube and calculate the optical conductivity of a nanotube.

To obtain this value, first let us find the electron wave functions for a model nanotube.

After the separation of variables in the Schrodinger equation written in cylindrical coordinates (ρ, φ, and z), we obtain, for an electron inside the nanotube, the following expression for the electron wave function:

$$\psi = \frac{\exp\left(ik_z z\right)}{\sqrt{L}} \frac{\exp\left(im\varphi\right)}{\sqrt{2\pi}} R_{mn}\left(\rho\right), \tag{1}$$

(here, n is a principal quantum number, k_z – wave-vector component connected with electron's motion along the $0z$ axis, m – integer, L – length of the cylinder; the cylinder occupies $[0, L]$ section of the $0z$ axis), in which the radial part R_{mn} satisfies the equation

$$\begin{cases} \frac{d^2 R_{mn}}{d\rho^2} + \frac{1}{\rho}\frac{dR_{mn}}{d\rho} + \left(\frac{2mE_\perp}{\hbar^2} - \frac{m^2}{\rho^2}\right) R_{mn} = 0, \\ \rho \in (a, b], \\ \frac{d^2 R_{mn}}{d\rho^2} + \frac{1}{\rho}\frac{dR_{mn}}{d\rho} + \left(\frac{2m(E_\perp - U_0)}{\hbar^2} - \frac{m^2}{\rho^2}\right) R_{mn} = 0, \\ \rho \notin (a, b], \end{cases} \tag{2}$$

here, $E_\perp$ is the energy connected with a transverse (relative to the $0z$ axis) motion:

$$E_\perp \equiv \frac{\hbar^2 k_\perp^2}{2m_e} = E - \frac{\hbar^2 k_z^2}{2m_e}, \tag{3}$$

$k_\perp$ – wave vector component associated with transversal motion of the electron, E – total electron energy, m_e – effective mass of the electron.

Solution of this equation is a linear combination of the Bessel and Neumann functions

$$R_{nm}(\rho) = B\left(\sin\alpha J_m\left(k_\perp \rho\right) + \cos\alpha N_m\left(k_\perp\rho\right)\right), \tag{4}$$

with α being some (constant) phase, B — constant factor (determined by the initial conditions), $\frac{\hbar^2 k_\perp^2}{2m_e} = E_\perp$, J_m — Bessel function of order m, N_m – Neumann function of order m.

We consider the electron to be localized in the potential well: $E_\perp < U_0$. Then we can apply, under the approximation of $k_\perp a \gg 1$, the Bessel functions' asymptotics on the interval $(a, b]$ as follows:

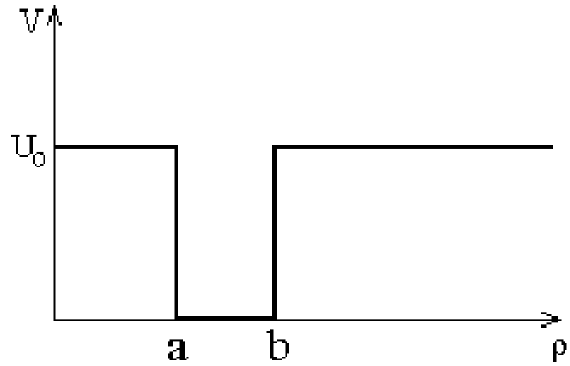

Fig. 1. Dependence of potential on the radial coordinate for model potential of a nanotube. U_0 — dielectric barrier height — is supposed to be equal in both the outside and the inside of a tube; a and b are inner and outer radii, respectively, of a nanotube; ρ is the radial coordinate of the cylindrical coordinate system

$$R_{nm} \approx B\left(\sin\alpha\sqrt{\frac{2}{\pi k_{nm}\rho}}\cos\left(k_{nm}\rho - \left(m+\frac{1}{2}\right)\frac{\pi}{2}\right) + \right.$$

$$\left. + \cos\alpha\sqrt{\frac{2}{\pi k_{nm}\rho}}\sin\left(k_{nm}\rho - \left(m+\frac{1}{2}\right)\frac{\pi}{2}\right)\right) =$$

$$= \frac{\tilde{B}}{\sqrt{\rho}}\sin\left(k_{nm}\rho - \left(m+\frac{1}{2}\right)\frac{\pi}{2} + \alpha\right), \tag{5}$$

where $\tilde{B} = \sqrt{\frac{2}{\pi k_{nm}}}B$. Beyond the range of the (a, b] interval, the asymptotics of Bessel functions is expressed as

$$R \approx \frac{C}{\sqrt{\rho}}\exp\left(-K_\perp\rho\right), \quad \rho > b; \quad R \approx \frac{A}{\sqrt{\rho}}\exp\left(K_\perp \rho\right),$$

$$\rho \le a, \quad K_\perp \rho >> 1, \tag{6}$$

where

$$\frac{\hbar^2 K_\perp^2}{2m_e} = U_0 - E_\perp, \tag{7}$$

with $K_\perp \gg k_\perp$. We proceed using the Kawabata and Kubo method [8]: since we suppose the barrier to be very high, at first we shall find a solution of Eq. (2) for an infinitely deep well ($U_0 \to \infty$) (unperturbed wave function), and then we shall calculate small corrections for the wave function parameters connected with the barrier finiteness.

Let us find, using the sewing condition, the spectrum of wave numbers (now we seek $k_\perp$ only) of the unperturbed wave function R^o. Since the barrier is considered to be infinitely high, we have

$$R^0(a) = R^0(b) = 0 \tag{8}$$

and, hence,

$$k_\perp(b-a) = \pi n, \qquad n \in Z, \tag{9}$$

from which we obtain the value of

$$k_\perp = k_n = \frac{\pi}{b-a} n \tag{10}$$

which is dependent on n only.

Let us find the normalization coefficient B. The normalization condition is

$$\int_0^L dz \int_0^{2\pi} d\varphi \int_a^b |\psi(\rho,\varphi,z)|^2 \rho d\rho = 1, \tag{11}$$

and, since the co-factors $\frac{\exp(ik_z z)}{\sqrt{L}}$ and $\frac{\exp(im\varphi)}{\sqrt{2\pi}}$ are already normalized on unity, we obtain

$$\int_a^b \left(R^0_{nm}(r)\right)^2 r dr = 1, \tag{12}$$

from where we get

$$\int_a^b \left(R^0_{nm}(r)\right)^2 r dr = \tilde{B}^2 \left(\frac{\rho}{2} - \frac{1}{4k_{nm}} \sin\left(2k_{nm}\rho - \right.\right.$$

$$\left.\left. -\left(m+\frac{1}{2}\right)\pi + 2\alpha\right)\right)\Bigg|_a^b = \tilde{B}^2 \frac{b-a}{2} = 1, \tag{13}$$

i.e.

$$\tilde{B} = \sqrt{\frac{2}{b-a}}. \tag{14}$$

Previously we have found, in accordance with formula (10), the wave vector component k_n transversal to the cylinder's longitudinal axis; this component rather exactly determines the electron spectrum, provided that the criterion $k_n a \gg 1$ is met. But this is not sufficient for us since we want to employ the method of Kawabata and Kubo [8] for the calculation of optical conductivity. In their approach, matrix elements of an optical transition are determined through the values of electron's radial functions on the boundary of the barrier. In approximation (10), these functions are equal to zero on the barrier's boundary. This is connected with the fact of taking the barrier's height to be infinite. If one considers the barrier of a limited height, a sewing should be done between the intra-well and intra-barrier values of the logarithmic derivative of the electron function. In this case, the boundary values of the wave function are nonzero and it becomes possible to find matrix elements of the optical transition. Thus, according to method [8], we proceed with the perturbed function. To do this, we introduce small corrections to k_n and α

$$k_\perp \to k_\perp + \Delta k_\perp, \quad \alpha \to \alpha + \Delta\alpha, \tag{15}$$

which can be found from the condition of logarithmic derivatives' sewing:

$$\frac{R'_{nm}(b+0)}{R_{nm}(b+0)} = \frac{R'_{nm}(b-0)}{R_{nm}(b-0)},$$
$$\frac{R'_{nm}(a+0)}{R_{nm}(a+0)} = \frac{R'_{nm}(a-0)}{R_{nm}(a-0)}. \tag{16}$$

For the wave function outside the (a,b] interval, we have

$$\rho \to b+0 \quad \frac{R'_{nm}(b+0)}{R_{nm}(b+0)} \approx -K_{nm}, \text{ since } K_{nl} b \gg 1,$$

$$\rho \to a-0 \quad \frac{R'_{nm}(a-0)}{R_{nm}(a-0)} \approx K_{nm}, \text{ since } K_{nl} a \gg 1;$$

and for that inside the (a,b] interval,

$$\frac{R'_{nm}(b-0)}{R_{nm}(b-0)} = \frac{k_{nm}\cos\pi m_1}{(\Delta k_{nm} b + \Delta\alpha)\cos\pi m_1} =$$
$$= \frac{k_{nm}}{\Delta k_{nm} b + \Delta\alpha},$$

because of equality to zero of the unperturbed wave function on the well boundaries $k_n b - \frac{\pi}{2}\left(m+\frac{1}{2}\right) + \alpha = \pi m_1$ with m_1 being some integer; analogously,

$$\frac{R'_{nm}(a+0)}{R_{nm}(a+0)} = \frac{k_n}{\Delta k_n a + \Delta\alpha},$$

hence

$$\begin{cases} \Delta k_n b + \Delta\alpha = -\frac{k_n}{K_n}, \\ \Delta k_n a + \Delta\alpha = \frac{k_n}{K_n}. \end{cases} \tag{17}$$

Thus, now we have an explicit form of the electron functions and the energy spectrum. We have not found an explicit form of α, but we need only a fact that "alpha" may be of a value that makes the unperturbed wave function vanish on the boundary of the potential well [we use this in Eq. (13)]. Now we can begin finding the optical conductivity proper; to calculate it, we need only linear combinations of Δk_n and $\Delta\alpha$ given in Eq. (17) instead of the properly Δk_n and $\Delta\alpha$ values, since there is no need to solve system (17).

2. Calculation of Optical Conductivity of a Nanotube

Now we are able to calculate nanotube's optical conductivity proper basing on the formula of Kawabata and Kubo [8]:

$$\sigma_1 = \frac{\pi e^2}{m_e^2 \omega^3 v_0} \sum_{(i,f)} \left| \langle i | \frac{\partial V}{\partial z} | f \rangle \right|^2 \times$$

$$\times f(E_i)(1 - f(E_f))\delta(E_f - E_i - \hbar\omega), \qquad (18)$$

here, σ_1 is the conductivity sought, ω – frequency of an incident photon, m_e – electron mass, v_0 – volume of the nanotube, $f(E)$ – the energy distribution electron function with the sum being taken over the initial i and final f states. (Note that hereinafter $f(E)$ denotes the energy distribution function, and index f – the final state; they are denoted by the same symbol.) The initial state $\langle i| = \langle k_z nm|$, $|f\rangle = |k_z' n' m'\rangle$; note that the expression under the summation sign does not depend in reality on m and m', in particular, the energy of the initial and the final states is, correspondingly, $E_i = E_{n,k_z}$, $E_f = E_{n',k_z'}$. Potential V is described by the formula

$$V = U_0 \left(\chi(\rho - b) - \chi(\rho - a) \right), \qquad (19)$$

in which $\chi(\rho)$ is the Heaviside function. Then

$$\frac{\partial V}{\partial z} = U_0(\delta(\rho - b) - \delta(\rho - a)) \cos\varphi, \qquad (20)$$

and a transition matrix element is

$$\langle i| \frac{\partial V}{\partial z} |f\rangle = U_0 \int_0^L \frac{\exp\left(i\left(k_z - k_z'\right) z\right)}{L} dz \times$$

$$\times \int_0^{2\pi} \frac{\exp\left(i\left(m - m'\right)\varphi\right)}{2\pi} \cos\varphi d\varphi \int_0^{+\infty} \rho(\delta(\rho - b) -$$

$$-\delta(\rho - a)) R^*_{nm}(\rho) R_{n'm'}(\rho) d\rho. \qquad (21)$$

Since we consider L to be of sufficiently large value, $\int_0^L \frac{\exp\left(i\left(k_z - k_z'\right)z\right)}{L} dz = \delta\left(k_z - k_z'\right)$, or, in a discrete form, $\delta_{k_z, k_z'}$; the factor

$$\int_0^{2\pi} \frac{\exp\left(i\left(m - m'\right)\varphi\right)}{2\pi} \cos\varphi d\varphi =$$

$$= \int_0^{2\pi} \frac{\exp\left(i\left(m - m'\right)\varphi\right)}{2\pi} \frac{e^{i\varphi} + e^{-i\varphi}}{2} d\varphi =$$

$$= \frac{1}{2}\left(\delta_{m,m'+1} + \delta_{m,m'-1}\right), \qquad (22)$$

and the integral over the radial variable

$$\int_0^{+\infty} \rho(\delta(\rho - b) - \delta(\rho - a)) R^*_{nm}(\rho) R_{n'm'}(\rho) d\rho =$$

$$= b R^*_{nm}(b) R_{n'm'}(b) - a R^*_{nm}(a) R_{n'm'}(a). \qquad (23)$$

By calculating the RHS part of this expression using Eq. (17), we obtain a final expression for the squared matrix element:

$$\left| < i | \frac{\partial V}{\partial z} | f > \right|^2 = \frac{2\hbar^4 \delta_{k_z,k_z'}}{m_e^2 (b-a)^2} \left(1 - (-1)^{n+n'}\right) \times$$

$$\times \frac{\delta_{m,m'-1} + \delta_{m,m'+1}}{2} k_n^2 k_{n'}^2, \qquad (24)$$

correspondingly, the conductivity

$$\sigma_1 = A \sum_{n,n',m,m',k_z,k_z'} \left(1 - (-1)^{n+n'}\right) \times$$

$$\times \delta_{k_z,k_z'} \frac{\delta_{m,m'-1} + \delta_{m,m'+1}}{2} k_n^2 k_{n'}^2 \times$$

$$\times f(E_{nm})(1 - f(E_{n'm'}))\delta(E_{nm} - E_{n'm'} - \hbar\omega) \qquad (25)$$

where

$$A = \frac{\pi e^2}{m_e^2 \omega^3 v_0} \frac{2\hbar^4}{m_e^2 (b-a)^2} = \frac{2\pi e^2 \hbar^4}{m_e^4 \omega^3 v_0 (b-a)^2} \qquad (26)$$

Since k does not depend on m, we can accomplish a summation over m. Issuing from general considerations (see, for instance, [5]), we have

$$m_{\max} = 2n. \qquad (27)$$

Therefore, the summation over m gives us

$$\sum_{m=0}^{2n} \frac{1}{2} = n. \qquad (28)$$

Analogously, for m', we obtain

$$\sum_{m'=0}^{2n'} \frac{1}{2} = n'. \qquad (29)$$

Let us draw our attention to the delta-indices $\delta_{m,m'+1}$ and $\delta_{m,m'-1}$. They bind the limits of summation over m and m': let an absorption take place (as in the case of our consideration)

$$E_f = E_i + \hbar\omega, \tag{30}$$

then (since $k_z = k'_z$ because of the presence of the factor δ_{k_z,k'_z})

$$(n')^2 = n^2 + n_\omega^2, \tag{31}$$

where

$$n_\omega^2 = \left(\frac{b-a}{\pi}k_\omega\right)^2 = \left(\frac{b-a}{\pi}\right)^2 \frac{2m_e}{\hbar^2}E_\omega =$$

$$= \left(\frac{b-a}{\pi}\right)^2 \frac{2m_e}{\hbar^2}\hbar\omega. \tag{32}$$

It follows from (31) that $n < n'$. Then the summation over m has to be performed from 0 to $2n$, and over m' – from 1 to $2n$+1, because of the presence of delta-index $\delta_{m,m'-1}$ in the co-factor $\frac{\delta_{m,m'-1}+\delta_{m,m'+1}}{2}$. Supposing that the addends with n=1 and n=2 contribute inessentially into the optical conductivity (i.e. $n \gg 1$), we can guess that the summation over m and m' is accomplished from 0 to $2n$, and the sum can be substituted as follows:

$$\sum_{m,m'} \frac{\delta_{m,m'-1} + \delta_{m,m'+1}}{2} \mapsto 2n = 2\frac{b-a}{\pi}k_\perp. \tag{33}$$

Therefore, the optical-conductivity sum will be written as

$$\sigma_1 = A \sum_{n,n',k_z,k'_z} \delta_{k_z,k'_z} 2\frac{b-a}{\pi}k_n \cdot \left(1 - (-1)^{n+n'}\right) k_n^2 k_{n'}^2 \times$$

$$\times f(E_{n,k_z})(1 - f(E_{n',k'_z}))\delta(E_{n,k_z} - E_{n',k'_z} - \hbar\omega). \tag{34}$$

While passing from summation to integration, the factor $1 + (-1)^{n+n'}$ may be replaced with its average value – unity. Then, for simplicity, we denote $k_n = k$, $k_{n'} = k'$, $E_i = E$, $E_f = E'$. Replacing the sum with an integral,

$$k = \frac{\pi}{b-a}n, \qquad k' = \tfrac{\pi}{b-a}n' \ , \tag{35}$$

$$k_z L = 2\pi n_z \tag{36}$$

(from the boundary conditions at the cylinder's ends), from where

$$\sum_{k_z} \to \frac{L}{2\pi}\int dk_z, \tag{37}$$

we obtain the sought optical conductivity in the zero approximation (we denote it as σ_1^0):

$$\sigma_1^0 = \frac{4\pi e^2\hbar^4}{m_e^4 (b-a)^2 \omega^3} \frac{1}{\pi (b^2 - a^2) L} \left(\frac{b-a}{\pi}\right)^2 \frac{L}{\pi} \left(\frac{b-a}{\pi}\right) \times$$

$$\times \int_{\Re} dk_z \int_0^\infty \int_0^\infty k^3 (k')^2\, dk dk' \times f(E)(1 - f(E')) \times$$

$$\times \delta(E - E' - \hbar\omega) = \frac{2e^2\hbar^4}{\pi^4 m_e^4 \omega^3} \frac{1}{b+a} \int_{\Re} dk_z \int_0^\infty \times$$

$$\times \int_0^\infty k^3 (k')^2\, dk dk' f(E)(1 - f(E'))\delta(E - E' - \hbar\omega). \tag{38}$$

The integral used in this expression is known from the calculation procedure of optical conductivity for a metallic cylinder [3]. We can write

$$\sigma_1^0 = \frac{3}{\pi^3} \frac{e^2 E_F^2}{\hbar^3 \omega^2} \frac{1}{b+a} g_c(\nu), \tag{39}$$

here, E_F is the Fermi energy, $\nu = \frac{\hbar\omega}{E_F}$, and

$$g_c(\nu) = \frac{16}{3\pi\nu} \int_{1-\nu}^{1} x^2 dx \int_0^1 \left(1 - y^2\right) \left(1 - y^2 + \frac{\nu}{y}\right)^{\frac{1}{2}} dy =$$

$$= \left(\frac{(x-\nu)(x+\nu)^2}{3\nu} - \frac{2}{3\pi\nu}(x-\nu)(x+\nu)^2 \times \right.$$

$$\left. \times \arcsin\left(\frac{\nu}{x+\nu}\right)^{\frac{1}{2}} + \frac{2}{3\pi}\left(\frac{x}{\nu}\right)^{\frac{1}{2}} \left(x^2 + \frac{2}{3}\nu x + \nu^2\right) \right) \Bigg|_{1-\nu}^{1} \tag{40}$$

Thus, formulae (39) and (40) give us the optical conductivity of a nanotube in the supposition of continuous spectrum (in our transition from sum (34) to integral (38), we have replaced the discrete spectrum of wave numbers with the continuous one). This approximation is admissible in the case of a non-thin-wall nanotube, otherwise, in the RHS of expression (39), one has to add a component connected with discreteness of the electron spectrum (it will be calculated in the next section).

3. Optical Conductivity Oscillations as a Manifestation of Electron Spectrum Quantization

In this section, we consider the effects associated with discreteness of the electron spectrum; they become noticeable in a thin-wall nanotube: $\frac{b-a}{a} << 1$.

We deal with the expression

$$\sigma_1 = 2A\frac{b-a}{\pi}\sum_{n,n',k_z}(1-(-1)^{n+n'})k_n^3 k_{n'}^2 f(E_{nm})\times$$

$$\times(1-f(E_{n'm'}))\delta(E_{nm}-E_{n'm'}-\hbar\omega), \qquad (41)$$

in which

$$A = \frac{2\pi e^2\hbar^4}{m_e^4\omega^3 v_0 (b-a)^2}, \qquad (42)$$

and, in the term $E_{n\prime m\prime}$ of Eq. (41), it is considered that $k_{z'} = k_z$.

Instead of the sum-to-integral replacement, Eqs. (35)—(37), we will use an exact summation formula, namely the Poisson formula:

$$\sum_{n=1}^{\infty} y(n) = \int_0^{\infty} dn\left(y(n) + 2\sum_{s=1}^{\infty} y(n)\cos(2\pi s n)\right). \qquad (43)$$

This procedure is used in the construction of the de Haas — van Alfven theory of oscillations (see, for example, [9]).

As regards to the summation over n with the Poisson formula, no difficulties arise. But, for the n' summation, some clarity and precautions need to be introduced.

So, we should calculate the sum

$$G\left(E(n)+\hbar\omega\right) \equiv \sum_{n'=1}^{\infty}\left(1-(-1)^{n+n'}\right)\times$$

$$\times\delta\left(E(n')-E(n)-\hbar\omega\right). \qquad (44)$$

The first notice is reduced to a statement that the delta function of discrete indices (n and n') makes no mathematical sense. To give a necessary sense to it, we have to recall that, in physics, the delta function represents some limit transition from a "normal" classical function (for example, of the C^∞ class' function or the one presented below). In the limit transition, the area bounded by the classical function remains to be equal to unity when its width (for example, at the half maximum) approaches zero and its height tends to infinity. As such a "normal" function, we take the function

$$\delta^*(x) = \begin{cases} 0, & x < -\frac{\Delta E}{2}, \\ \frac{1}{\Delta E}, & -\frac{\Delta E}{2} < x < \frac{\Delta E}{2}, \\ 0, & x > \frac{\Delta E}{2} \end{cases} \qquad (45)$$

with $\Delta E \to 0$.

The second notice concerns the function $\left(1-(-1)^{n'+n}\right)$ which takes a value of 0 or 2 depending on the evenness or oddness of $n'+n$. In the previous section, we have replaced this function with its average value (unity). If one accounts for the spectrum discreteness, this approximation becomes doubtful. But justification of this approximation can be proved strictly if, in Eq. (44), one separately considers the situations of even and odd values of n. Let us suppose, for example, that n takes only odd values in Eq. (44). Then only even values of $n' = 2p'$ (with $p' = 1, 2, 3, ...$) remain in the sum. Therefore, in this case,

$$G\left(E(n)+\hbar\omega\right) = 2\sum_{p'=1}^{\infty}\delta^*\left(E(2p')-E(n)-\hbar\omega\right). \qquad (46)$$

Now let us apply Eq. (43) to the summation in (46):

$$G\left(E(n)+\hbar\omega\right) = \int_0^{\infty} dp'\cdot 2\delta^*\left(E\left(2p'\right)-E(n)-\hbar\omega\right)\times$$

$$\times\left(1+2\sum_{s=1}^{\infty}\cos\left(2\pi s\cdot 2p'\right)\right) =$$

$$= \int_0^{\infty} dn'\delta^*\left(E\left(n'\right)-E(n)-\hbar\omega\right)\left(1+2\sum_{s=1}^{\infty}\cos\left(2\pi s n'\right)\right).$$

We can see that the obtained result coincides with the initial one obtained after the replacement of $\left(1-(-1)^{n+n'}\right)$ by unity. A similar substantiation may be done for even values of n; in this case, only odd values of n' (that is $n' = 2m'-1$) contribute to the sum.

Thus, in Eq. (44), we replace the discrete function $\left(1-(-1)^{n+n'}\right)$ by its average value, unity, and the delta function – by δ^*, and apply the Poisson formula to the obtained sum. We get

$$G\left(E+\hbar\omega\right) = \frac{(b-a)\sqrt{2m_e}}{2\pi\hbar\sqrt{E+\hbar\omega}}\times$$

$$\times\left(1+2\sum_{s=1}^{\infty}\cos\left(s\frac{2\,(b-a)}{\hbar}\sqrt{2m_e\left(E+\hbar\omega\right)}\right)\right). \qquad (47)$$

For simplicity, we omit the dependence of E on n in Eq. (47). Besides this, in obtaining Eq. (47), we already have accomplished the passage to the limit $\Delta E \to 0$ (here, ΔE is the same as in Eq. (45)). Let us substitute $G(E+\hbar\omega)$ into expression (41) and apply once more Eq. (43) for taking the sum over n. We obtain

$$\sigma_1 = \frac{4\pi e^2\hbar^4}{m_e^4 (b-a)^2 \omega^3} \frac{1}{\pi (b^2-a^2) L} \left(\frac{b-a}{\pi}\right)^2 \frac{L}{2\pi} \times$$

$$\times \left(\frac{b-a}{\pi}\right) \int_0^\infty dk_z \int_0^\infty \int_0^\infty dk dk' k^3 (k')^2 \times$$

$$\times f(E)(1-f(E'))\delta(E-E'-\hbar\omega) = \frac{2e^2\hbar^4}{\pi^4 m_e^4 \omega^3} \frac{b-a}{b^2-a^2} \times$$

$$\times \int_0^\infty dk_z \int_0^\infty \int_0^\infty dk dk' k^3 (k')^2 f(E)(1-f(E+\hbar\omega))\delta(E-$$

$$-E'-\hbar\omega) \left(1 + 2\sum_{s=1}^\infty \cos\left(s\frac{2(b-a)}{\hbar}\sqrt{2m_e E(k,k_z)}\right)\right) \times$$

$$\times \left(1 + 2\sum_{s'=1}^\infty \cos\left(s'\frac{2(b-a)}{\hbar}\sqrt{2m_e (E(k,k_z)+\hbar\omega)}\right)\right) =$$

(it follows from $k_z = k_z'$ that $(k')^2 = \frac{2m}{\hbar^2}(E_\perp + \hbar\omega)$; we execute the integration of the delta function)

$$= \frac{2e^2\hbar^4}{\pi^4 m_e^4 \omega^3} \frac{1}{b+a} \left(\frac{2m_e}{\hbar^2}\right)^{\frac{3}{2}} \left(\frac{m_e}{\hbar^2}\right)^2 \int_0^\infty dk_z \int_0^\infty dE_\perp E_\perp \times$$

$$\times \sqrt{E_\perp + \hbar\omega} f(E)(1-f(E+\hbar\omega)) \times$$

$$\times \left(1 + 2\sum_{s=1}^\infty \cos\left(s\frac{2(b-a)}{\hbar}\sqrt{2m_e E}\right)\right) \times$$

$$\times \left(1 + 2\sum_{s'=1}^\infty \cos\left(s'\frac{2(b-a)}{\hbar}\sqrt{2m_e (E+\hbar\omega)}\right)\right). \quad (48)$$

Estimations show that, for $b - a \geq 2\cdot 10^{-7}$ cm and with the energy values of about the order of magnitude of the Fermi energy, the cosine arguments in Eq. (48) are far more than unity. This implies that the cosines in Eq. (48) are fast oscillating functions of energy. Hence, only components with $s = s'$ and those including a difference between the arguments of two cosines make a considerable contribution:

$$\varphi_s(E) \equiv s\frac{2(b-a)}{\hbar}\sqrt{2m_e}\left(\sqrt{E+\hbar\omega} - \sqrt{E}\right). \quad (49)$$

These are the components that possess a minimal frequency of oscillations and, therefore, their contribution to the integral Eq. (48) becomes dominating.

Retaining in Eq. (48) only the terms of Eq. (49) type, we obtain

$$\sigma_1 = \frac{8e^2}{\pi^4\omega^3\hbar^3\sqrt{2m_e}} \frac{1}{b+a} \int_0^{+\infty} \frac{dp_z}{\hbar} \int_0^\infty dE_\perp E_\perp \sqrt{E_\perp + \hbar\omega} \times$$

$$\times f(E)(1-f(E+\hbar\omega)) \left(1 + 2\sum_{s=1}^\infty \cos\varphi_s(E)\right) = \sigma_1^0 +$$

$$+ \frac{16e^2}{\pi^4\omega^3\hbar^4\sqrt{2m_e}} \frac{b-a}{b^2-a^2} \int_0^{+\infty} dp_z \int_0^\infty dE_\perp E_\perp \sqrt{E_\perp + \hbar\omega} \times$$

$$\times f(E)(1-f(E+\hbar\omega)) \sum_{s=1}^\infty \cos\varphi_s(E) \quad (50)$$

($p_z = \hbar k_z$, σ_1^0 is given by expression (39)).

So we came to the known integral (see the analogous calculation in [5]):

$$\int_0^{+\infty} dp_z \int_0^\infty E_\perp \sqrt{E_\perp + \hbar\omega} dE_\perp f(E)(1-f(E+\hbar\omega)) \times$$

$$\times \sum_{s=1}^\infty \cos\varphi_s(E) = \frac{3}{2}\pi^{\frac{3}{2}} E_{\rm F}\theta\hbar\omega\sqrt{2m_e}\Bigg(1-$$

$$-\exp\left(-\frac{\hbar\omega}{\theta}\right)\Bigg)^{-1} \sum_{s=1}^\infty \frac{\cos(\varphi_s(E_{\rm F}) - \frac{\pi}{4})}{\sqrt{E_{\rm F}|\varphi_s'(E_{\rm F})|}\,\mathrm{sh}(\pi\theta\varphi_s'(E_{\rm F}))}, \quad (51)$$

here, $E_{\rm F}$ – Fermi energy, θ – temperature; from this, we obtain for optical conductivity as

$$\sigma_1 = \sigma_1^0 + \frac{16e^2}{\pi^4\omega^3\hbar^4\sqrt{2m_e}} \frac{1}{b+a} \cdot \frac{3}{2}\pi^{\frac{3}{2}} E_{\rm F}\theta\hbar\omega\sqrt{2m_e}\Bigg(1-$$

$$-\exp\left(-\frac{\hbar\omega}{\theta}\right)\Bigg)^{-1} \sum_{s=1}^\infty \frac{\cos\left(\varphi_s(E_{\rm F}) - \frac{\pi}{4}\right)}{\sqrt{E_{\rm F}|\varphi_s'(E_{\rm F})|}\,\mathrm{sh}\left(\pi\theta\varphi_s'(E_{\rm F})\right)} =$$

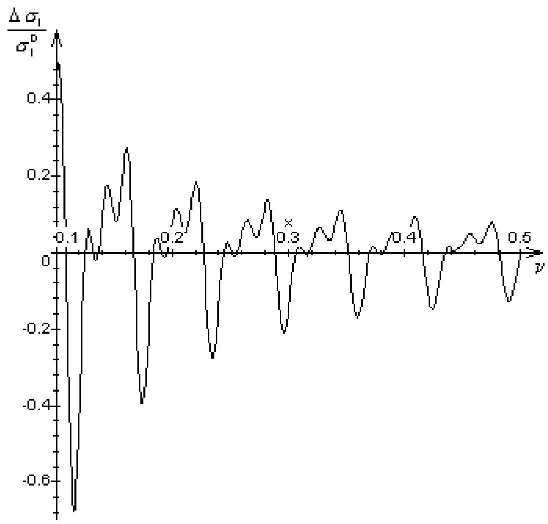

Fig. 2. Dependence of d on ν for $E_{\mathrm{F}} = 5.53$ eV, $T = 300$ K, $b - a = 10$ nm

$$= \sigma_1^0 + \frac{24e^2}{\pi^{\frac{5}{2}}\hbar^3\omega^2} E_{\mathrm{F}}\theta \frac{1}{b+a}\left(1 - \exp\left(-\frac{\hbar\omega}{\theta}\right)\right)^{-1} \times$$

$$\times \sum_{s=1}^{\infty} \frac{\cos\left(\varphi_s(E_{\mathrm{F}}) - \frac{\pi}{4}\right)}{\sqrt{E_{\mathrm{F}}|\varphi_s'(E_{\mathrm{F}})|}\mathrm{sh}\left(\pi\theta\varphi_s'(E_{\mathrm{F}})\right)} = \sigma_1^0 + \Delta\sigma_1, \quad (52)$$

where

$$\Delta\sigma_1 = \frac{24e^2}{\pi^{\frac{5}{2}}\hbar^3\omega^2} E_{\mathrm{F}}\theta \frac{1}{b+a}\left(1 - \exp\left(-\frac{\hbar\omega}{\theta}\right)\right)^{-1} \times$$

$$\times \sum_{s=1}^{\infty} \frac{\cos\left(\varphi_s(E_{\mathrm{F}}) - \frac{\pi}{4}\right)}{\sqrt{E_{\mathrm{F}}|\varphi_s'(E_{\mathrm{F}})|}\mathrm{sh}\left(\pi\theta\varphi_s'(E_{\mathrm{F}})\right)}.$$

If we take room temperature $T = 300$ K, then it can be seen that the factor $\left(1 - \exp\left(-\frac{\hbar\omega}{\theta}\right)\right)^{-1}$ does not affect noticeably the result obtained for practical $\hbar\omega$ values (say, for a CO_2 laser, the $\hbar\omega$ value is about 0.1 eV, then $\frac{\hbar\omega}{\theta} = 5.31$ and $\left(1 - \exp\left(-\frac{\hbar\omega}{\theta}\right)\right)^{-1} \approx 0.995$). So, this factor can be neglected and, with accounting for (39), we can write

$$\sigma_1 = \sigma_1^0 + \frac{24e^2}{\pi^{\frac{5}{2}}\hbar^3\omega^2} E_{\mathrm{F}}\theta \frac{1}{b+a} \times$$

$$\times \sum_{s=1}^{\infty} \frac{\cos\left(\varphi_s(E_{\mathrm{F}}) - \frac{\pi}{4}\right)}{\sqrt{E_{\mathrm{F}}|\varphi_s'(E_{\mathrm{F}})|}\mathrm{sh}\left(\pi\theta\varphi_s'(E_{\mathrm{F}})\right)} =$$

$$= \sigma_1^0 \left(1 + 8\sqrt{\pi}\frac{\theta}{E_{\mathrm{F}}} \frac{\sum_{s=1}^{\infty} \frac{\cos\left(\varphi_s(E_{\mathrm{F}}) - \frac{\pi}{4}\right)}{\sqrt{E_{\mathrm{F}}|\varphi_s'(E_{\mathrm{F}})|}\mathrm{sh}\left(\pi\theta\varphi_s'(E_{\mathrm{F}})\right)}}{g_c(\nu)}\right) \quad (53)$$

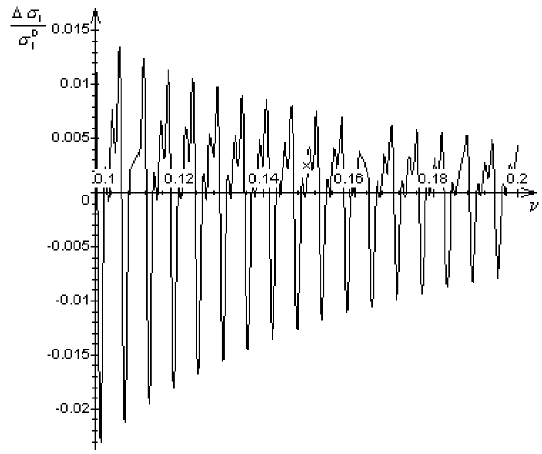

Fig. 3. Dependence of d on ν for $E_{\mathrm{F}} = 5.53$ eV, $T = 300$ K, $b - a = 100$ nm

or, if we introduce

$$q_0(\nu) \equiv \frac{2(b-a)}{\hbar}\sqrt{2m_e E_{\mathrm{F}}}\left(\sqrt{1+\nu} - 1\right) = \frac{\varphi_s(E_{\mathrm{F}})}{s} \quad (54)$$

and

$$q_1(\nu) \equiv \frac{b-a}{\hbar}\sqrt{\frac{2m_e}{E_{\mathrm{F}}}}\left(\frac{1}{\sqrt{1+\nu}} - 1\right) = \frac{\varphi_s'(E_{\mathrm{F}})}{s}, \quad (55)$$

then, finally, we can write

$$\sigma_1 = \sigma_1^0\left(1 + 8\sqrt{\pi}\frac{\theta}{E_{\mathrm{F}}}F(\nu)\right), \quad (56)$$

where

$$F(\nu) = \frac{\sum_{s=1}^{\infty} \frac{\cos\left(sq_0(\nu) - \frac{\pi}{4}\right)}{\sqrt{sE_{\mathrm{F}}|q_1(\nu)|}\mathrm{sh}\left(\pi\theta q_1(\nu)\right)}}{g_c(\nu)}. \quad (57)$$

Our calculations show that, for $b - a > 10$ nm, there is enough to take three terms in the sum over s. In Fig. 2, the curve shows the ratio of the oscillating correction (with retaining the three terms) to the optical conductivity of zero approximation, expressed by the function $d(\nu) \equiv \frac{\Delta\sigma_1}{\sigma_1^0} = 16\sqrt{\pi}\frac{\theta}{E_{\mathrm{F}}}F(\nu)$, for parameters $E_{\mathrm{F}} = 5.53$ eV (Fermi energy of Au), $T = 300$ K, and $b - a = 10$ nm.

The analogous curve for $b - a = 100$ nm is presented in Fig. 3.

Thus, we have obtained the optical conductivity of a metallic nanotube without limitations on its thickness, i.e. without applying the condition $k_n(b-a) \gg 1$; it was sufficient to use the inequality $k_n a \gg 1$. This gives us grounds for the calculation of the optical conductivity of a nanotube with a wider variety of its parameters. We can see that the discrete-electronic-spectrum addend in the optical-conductivity expression is an oscillating function of the energy of a photon incident onto the nanotube; in this case, as is seen from a comparison between Fig. 1 and Fig. 2, the dependence of the oscillating addend on nanotube's thickness is essential.

Summary and Remarks

Thus, we have obtained an expression for the optical conductivity of a metallic nanotube without taking the electron energy spectrum quantization into account (we can see that the expression transforms, when the inner radius tends to zero, into the known formula for a solid metallic cylinder [3]); we also have found an approximate expression for the small addend to optical conductivity connected with quantization of the electron energy spectrum (the effect manifests itself in thin nanotubes). The dependence of this addend on the energy of an incident electromagnetic wave shows oscillations; moreover, a change of the nanotube's thickness essentially affects the shape of these oscillations. The obtained result transforms into the known expression for the optical conductivity of thin metallic wires [3,8] if the inner diameter of a tube tends to zero. As was expected, we can see that, with fixing any of the nanotube's radii (say, the inner one) and varying the other (outer), we can employ the asymptotics of radial wave functions by varying the interlevel electron-energy gaps in a wide range.

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ОПТИЧНА ПРОВІДНІСТЬ МЕТАЛЕВИХ НАНОТРУБОК

П.М. Томчук, Вол.В. Куліш

Р е з ю м е

Отримано явний вираз для залежності оптичної провідності металевої нанотрубки від внутрішнього і зовнішнього радіусів нанотрубки і відношення енергії фотона до енергії Фермі. Знайдено явний вигляд поправки до оптичної провідності, зумовленої квантуванням енергії електрона в металевій нанотрубці; визначено осциляційний характер залежності цієї поправки від частоти світла.