One-dimensional semirelativity for electrons in carbon nanotubes

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It is shown that the band structure of single-wall semiconducting carbon nanotubes (CNT) is analogous to relativistic description of electrons in vacuum, with the maximum velocity $u=10^8$ cm/s replacing the light velocity. One-dimensional semirelativistic kinematics and dynamics of electrons in CNT is formulated. Two-band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian is employed to demonstrate that electrons in CNT experience a zitterbewegung (trembling motion) in absence of external fields. This zitterbewegung should be observable much more easily in CNT than its analogue for free relativistic electrons in vacuum. It is argued that in the lowest subband of metallic CNT, where the rest effective mass of electrons vanishes, the zitterbewegung should not occur.

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I. INTRODUCTION

Since the first reported observations of carbon nanotubes[1,2] these unique one-dimensional nanostructures were subject of very intensive research, both because of their remarkable properties as well as their potential use in nanometer-sized electronics (see Refs. 3 and 4). Among other particularities carbon nanotubes (CNT) have an interesting energy band structure and it is this aspect that is of our concern here. We will be interested in the simplest single-wall semiconducting and metallic CNT. Such tubes are obtained from a slice of graphene wrapped into a seamless cylinder, so that the one-dimensional (1D) band structure of CNT can be constructed by using the two-dimensional (2D) band structure of graphene. The periodic boundary condition around the tube circumference causes quantization of the transverse wave vector component k_x. The purpose of our work is to predict new properties of electrons and holes in CNT in the classical and quantum domains. To this end we use a similarity of the band structure of CNT to the relativistic description of free electrons in vacuum. In particular, we predict that the "semirelativistic" band structure of semiconducting CNT should result in a zitterbewegung (trembling motion) of nonrelativistic electrons in absence of external fields. Similar phenomenon was predicted for relativistic electrons in vacuum but never observed. Thus, an observation of the zitterbewegung in CNT would be of great importance not only for the solid state physics but also for the high energy physics.

II. SEMIRELATIVITY

In the following we use the $\mathbf{k}\cdot\mathbf{p}$ band structure at the K point of the Brillouin zone.[5,6] This band structure is well established in the vicinity of the Fermi energy. The initial 2×2 Hamiltonian is written in the form

$$\hat{H}=\alpha\begin{bmatrix}0 & a_n-i\hat{p}\\ a_n+i\hat{p} & 0\end{bmatrix}, \tag{1}$$

where α is a coefficient, $\hat{p}$ is the operator of pseudomomentum in the y direction and a_n is given by the quantization of the wave vector k_x. There is $a_n=\hbar k_x(n)=\hbar(2\pi/L)(n-\nu/3)$ for $n=0,\pm1,\pm2,\ldots$. Here L is the length of circumference. The semiconducting CNT of our interest are obtained for $\nu=\pm1$. In absence of external fields the resulting energy is $\mathcal{E}=\pm E(p)$, where $E(p)=\alpha(a_n^2+p^2)^{1/2}$. The upper sign is for the conduction and the lower for the valence band. The above relation is analogous to the dispersion $E(p)$ for free relativistic electrons in vacuum. We write the energy in the following equivalent form:

$$E(p)=\left[\left(\frac{\epsilon_g}{2}\right)^2+\epsilon_g\frac{p^2}{2m_0^*}\right]^{1/2}, \tag{2}$$

where $\epsilon_g=2\alpha a_n$ is the energy gap and $m_0^*=a_n/\alpha$ is the effective mass at the band edge, related to band's curvature for small p values. Both ϵ_g and m_0^* have different values for different subbands n. Equation (2) has the relativistic form with the correspondence $\epsilon_g\to 2m_0c^2$ and $m_0^*\to m_0$.[7]

We first investigate some consequences of the one-dimensional dispersion (2). The electron velocity is $v=dE/dp=\alpha^2p/E$. For large momenta the velocity reaches a saturation value $u=\alpha=(\epsilon_g/2m_0^*)^{1/2}$, the same for all subbands. The maximum velocity u plays for electrons in CNT the role of the light velocity c for relativistic electrons in vacuum. Using u we can write the energy in another equivalent form

$$E(p)=\left[(m_0^*u^2)^2+u^2p^2\right]^{1/2}, \tag{3}$$

which is directly reminiscent of the relativistic $E(p)$ relation. Now we define an energy-dependent effective mass m^* relating velocity to momentum

$$m^*v=p. \tag{4}$$

We calculate $m^*=p/v=E/u^2$. This gives

$$E=m^*u^2, \tag{5}$$

which is in one-to-one correspondence to the Einstein relation $E=mc^2$ (the maximum velocity u replacing c). For $p=0$ Eqs. (3) and (5) reduce to $E_r=m_0^*u^2$, which corresponds to the formula for the rest energy. One can also express the mass m^* by the velocity. Beginning with the relation $p^2u^2=v^2E^2/u^2$, employing $E^2=(m_0^*u^2)^2+u^2p^2$ and solving for momentum, we get

$$p = m_0^* \gamma v, \tag{6}$$

where $\gamma=(1-v^2/u^2)^{-1/2}$. Using the above definition $p=m^*v$ we have $m^*=m_0^*\gamma$, which has the familiar relativistic form (with u replacing c). Now Eq. (5) reads $E=m_0^*\gamma u^2$.

Next we assume, in analogy with the special relativity, that $dp/dt=F$, where F is the force. One can now define another effective mass M^*, relating force to acceleration

$$M^* a = F. \tag{7}$$

Since $a=dv/dt=(dv/dp)(dp/dt)=(d^2E/dp^2)F$, we obtain $1/M^*=d^2E/dp^2$. Using the above dispersion $E(p)$ we obtain

$$M^* = \frac{E^3}{m_0^{*2}u^6} = m_0^* \gamma^3, \tag{8}$$

which again has the corresponding relation in special relativity if the acceleration is parallel to the force.

Estimating the introduced quantities, we use the value of $\alpha\hbar=6.46$ eV Å.[6] This gives for the maximum velocity $u=\alpha=0.98\times10^8$ cm/s, which shows explicitly that we deal with nonrelativistic electrons. The lowest energy gap is $\epsilon_g(0)=2\alpha a_0$, where $a_0=\hbar 2\pi/3L$. For the circumference $L=60$ Å we get $\epsilon_g(0)=0.45$ eV. The effective mass $m_0^*/m_0=a_0/\alpha m_0=0.041$ for the same conditions. The quoted parameters are close to those of the typical narrow gap semiconductor InAs, but CNT of higher diameter have smaller ϵ_g and m_0^*. We emphasize that, while for a nonparabolic energy band one can legitimately define both energy dependent masses m^* and M^*, it is the "momentum" mass m^* that is a more useful quantity. This mass is employed in the transport theory since the current is related to velocity, not to acceleration. It is m^* that enters into the equivalence of the mass and the energy in Eq. (5). Finally, m^* is related to the density of electron states since the latter is $\rho(E)=(1/\pi\hbar)(dp/dE)=(1/\pi\hbar)(m^*/p)$. We emphasize that, even if other energy levels had to be included in the kp theory, the first nonparabolic approximation to the dispersion relation is always of the type given by Eq. (2). The only difference is that ϵ_g in Eq. (2) is then replaced by an effective gap.

III. ZITTERBEWEGUNG

Next we consider the quantum effects in CNT related to the Hamiltonian (1). To this purpose we introduce an important quantity[8]

$$\lambda_Z = \frac{\hbar}{m_0^* u} = \frac{\hbar}{a_n}, \tag{9}$$

which we call the length of zitterbewegung (see below). It corresponds to the Compton wavelength λ_c for electrons in vacuum and it plays for the semirelativistic band structure (1) the role that λ_c does for the Dirac equation. However, λ_Z is several orders of magnitude larger than λ_c. Using $m_0^*=0.041m_0$ and $u=0.98\times10^8$ cm/s we calculate $\lambda_Z=28.6$ Å.

Now let us consider the operator of electron velocity $\hat{v}=d\hat{H}/d\hat{p}$. A simple calculation shows that the eigenvalues of $\hat{v}$ are, paradoxically, $\pm u$. This differs drastically from the classical velocity calculated above. To clear the paradox we calculate $\hat{v}(t)$. Using Eq. (1) we get $\hat{v}\hat{H}+\hat{H}\hat{v}=2\alpha^2\hat{p}=2u^2\hat{p}$. Hence the time derivative of $\hat{v}$ is

$$\frac{d\hat{v}}{dt} = \frac{i}{\hbar}2u^2\hat{p} - \frac{2i}{\hbar}\hat{v}\hat{H}. \tag{10}$$

This represents a simple differential equation for $\hat{v}$. Its solution is

$$\hat{v}(t) = \frac{u^2}{\hat{H}}\hat{p} + \left(\hat{v}_0 - \frac{u^2\hat{p}}{\hat{H}}\right)\exp\left(-2i\frac{\hat{H}t}{\hbar}\right), \tag{11}$$

where $1/\hat{H}=E^{-2}\hat{H}$. Thus the quantum velocity differs from the classical one by the term that oscillates in time. Equation (11) can be integrated with respect to time to give the position operator $\hat{y}$ in the Heisenberg picture

$$\hat{y}(t) = \hat{y}(0) + \frac{u^2\hat{p}}{\hat{H}}t + \frac{i\hbar u}{2\hat{H}}\hat{A}_0\left[\exp\left(\frac{-2i\hat{H}t}{\hbar}\right) - 1\right], \tag{12}$$

where $\hat{A}_0=(\hat{v}_0/u)-(u\hat{p}/\hat{H})$. The first two terms of Eq. (12) represent the classical electron motion. The third term describes time-dependent oscillations with the frequency $\omega_Z=\epsilon_g/\hbar$. Since $\hat{A}_0\approx1$ the amplitude of oscillations is $2\hbar u/2\hat{H}\approx\hbar/m_0^*u=\lambda_Z$. In the relativistic quantum mechanics (RQM) of free electrons the analogous oscillations were devised by Schrödinger,[9,10] who called them zitterbewegung (ZB). This explains the name given above to λ_Z. We note that the phenomenon of ZB goes beyond Newton's first law since we have a nonconstant velocity without a force. In RQM it is demonstrated that the ZB is a result of interference between the states of positive and negative electron energies.[11] The ZB described above for CNT has the frequency of about 10^7 times lower and the amplitude of about 10^4-10^5 times higher than the corresponding values for relativistic electrons in vacuum. We come back to the problem of ZB below.

In order to investigate the case of a definite sign of energy we complete the Hamiltonian (1) by the potential $V(y)$ on the diagonal and introduce magnetic field by adding a vector potential to the momentum operator. We then try to separate the 2×2 eigenenergy problem employing the Hamiltonian (1) into two independent problems for each band. This can be easily done in the semiclassical approximation neglecting the noncommutativity of $\hat{p}$ with V. One obtains then, as expected, the one-band effective mass approximations for the conduction and valence bands

$$\hat{H} = \pm\frac{\epsilon_g}{2} \pm \frac{\hat{P}^2}{2m_0^*} + V, \tag{13}$$

where $\hat{P}=\hat{p}_y+eA_y$ is the canonical momentum.

In absence of external potentials the two-component wave functions resulting from the Hamiltonian (1) can be transformed exactly into one-component functions for positive (or negative) electron energies. This is achieved by applying the following unitary transformation $\hat{S}$:

$$\hat{S} = \frac{1}{\sqrt{2}}\left(1 + \frac{\hat{\beta}\hat{H}}{E}\right), \tag{14}$$

where $\hat{\beta}=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$. It can be verified that $\hat{S}\hat{S}^{+}=1$ and that the transformed Hamiltonian $\hat{H}_{\phi}$ is

$$\hat{H}_{\phi} = \hat{S}\hat{H}\hat{S}^{+} = E\hat{\beta}. \tag{15}$$

Thus the positive and negative energies are separated. One can transform any wave function $\psi(y')$ [not only the eigenfunctions of the Hamiltonian (1)] from the original two-component representation to the one-component ϕ representation by the following integral transformation (cf. Refs. 12–14):

$$\psi'_{\pm}(y) = \int K_{\pm}(y,y')\psi(y')dy', \tag{16}$$

where

$$K_{\pm}(y,y') = \frac{1}{8\pi}(1 \pm \hat{\beta}) \int \left(1 \pm \frac{\hat{H}}{E_p}\right) e^{ip'(y-y')}dp'. \tag{17}$$

The subscripts $\pm$ correspond to the one-component functions related to positive or negative energy, respectively. The factors $(1\pm\hat{\beta})$ guarantee this property. The kernels $K_{\pm}(y,y')$ are not point transformations. Suppose we are interested in the eigenfunction of the electron position $\hat{y}$. It is convenient to take in the initial representation the unit vector $\psi(y')=\binom{1}{0}\delta(y'-y_0)$, where δ is the Dirac delta function. It follows then from Eq. (16) that the transformed one-component functions are $K_{\pm}(y-y_0)$. The integrals of $K_{\pm}(y-y_0)$ over $Y=y-y_0$ are unity. To get an idea of the extension of $K_{\pm}(y-y_0)$ we calculate their second moment. After some manipulation we obtain

$$\int Y^2 K_{\pm}(Y)dY = \tfrac{1}{2}\lambda_Z^2. \tag{18}$$

Thus the extension of the transformed eigenfunctions of position is $|y-y_0|=\lambda_Z/\sqrt{2}$. In the transformed states there is no ZB since the transformation (14) [or (16)] eliminates the negative (positive) energy components of the wave functions. Following the interpretation established in RQM we are confronted with the choice between a pointlike electron described by a two-component function (four components including spin) which experiences the ZB with the amplitude of λ_Z, and an electron described by a one-component function (two components including spin) for either positive (or negative) electron energy which does not experience the ZB but is "smeared" in the y direction to an object of the size λ_Z. One can say that in the one-component representation the trembling motion is averaged into smearing. As follows from the above estimation of λ_Z, the amplitude of ZB or, alternatively, the smearing of electrons in CNT is quite large and it should be observable directly or indirectly.

IV. DISCUSSION

In a recent paper[15] zitterbewegung-type oscillations were proposed using the Hamiltonian of spin splitting due to structure inversion asymmetry (SIA) or bulk inversion asymmetry (BIA) of the system.[16–18] The Hamiltonian for BIA has the form $\hat{H}_D=(\beta/\hbar)(\sigma_y\hat{p}_y-\sigma_x\hat{p}_x)$, where σ_x and σ_y are the Pauli spin matrices. Interestingly, the Hamiltonian (1) which we use for CNT has the identical form, with the minus sign in $\hat{H}_D$ replaced by the plus sign in Eq. (1). This similarity is formal because the Hamiltonian (1) is not related to spin. The description of Ref. 15 begins with a 2D case but finally treats a quantum wire, which is a system almost identical with CNT. Considering the motion of a wave packet it shows that the ZB occurs in the direction perpendicular to the packet's group velocity. Its frequency is $\omega=\Delta E/\hbar$, where ΔE is the energy splitting, and its amplitude is inversely proportional to the packet's wave vector. Our Eq. (12) describes the same result for the frequency, namely $\omega_Z=\epsilon_g/\hbar$. As to the amplitude, our result is also the same since the ZB in the y direction has the amplitude $\lambda_Z=\hbar/a_n=1/k_x(n)$, where $k_x(n)$ is the wave vector in the x direction. However, in our case, for each $k_x(\nu,n)$ there exists $k_x(-\nu,-n)=-k_x(\nu,n)$, resulting in two degenerate subbands, and the ZBs related to these subbands will cancel each other. The easiest way to break this symmetry is to apply an external magnetic field parallel to the tube axis. Such a field changes the phase factor in the wave function leading to $k_x=(2\pi/L)(n-\nu/3+\phi/\phi_0)$, where ϕ is the magnetic flux and $\phi_0=ch/e$ is the flux quantum, see Ref. 6. The magnetic term breaks the above symmetry and the cancellation of the two trembling motions will not occur.

As compared to the oscillatory electron motion proposed in Ref. 15, the ZB in CNT described above has an important advantage. Namely, the ZB of electrons in CNT is the "true" zitterbewegung in a sense that it corresponds to the ZB for free relativistic electrons in vacuum, while the oscillatory motion proposed in Ref. 15 has no such correspondence. Thus the observation of ZB in CNT would be of great value also for the relativistic quantum mechanics. There exist in the literature contradictory statements concerning the observability of ZB in vacuum (see, e.g., Refs. 10, 19, and 20), which makes its analogue in solids and molecules even more interesting.

The ZB described above can be observed with the use of scanning probe microscopy (SPM), which is able to image coherent electron flow.[21,22] The SPM uses a movable tip that, properly biased, probes the electron density below it. As the zitterbewegung changes the electron density along the tube's circumference, it will induce oscillations of the tube's conductance when the tip is moved along the circumference. A specific way, particular to the CNT geometry, could possibly be used. As mentioned above, without an external magnetic field the two components of ZB corresponding to the two directions of the quantized transverse momentum cancel each other. This means that switching on a magnetic field "triggers" the appearance of the net ZB motion. In consequence, after the magnetic field is switched on a charge begins to flow along the free direction y, that is *parallel* to magnetic field. This could serve as a signature of the ZB since the usual effect of a magnetic field is to affect the motion *transverse* to magnetic field. A single wall CNT is a particularly favorable system since the ZB occurs on the surface, in which case the SPM imaging of the electron wave

function is relatively easy. It should be mentioned that the scanning probe microscopy was already successfully applied to CNT.[23–25]

Finally, we briefly consider the case of metallic CNT. In our notation of Eq. (1) the metallic CNT are characterized by the quantum number $\nu=0$, which gives $a_0=0$ for $n=0$. This leads to $\mathcal{E}=\pm E(p)$, where $E(p)=\alpha|p|$. This means that for the lowest subband there is no energy gap. The maximum velocity u can still be defined, there is, as before, $u=\alpha$. In fact, the classical velocity is *always* u. The rest effective mass vanishes, $m_0^*=a_n/\alpha=0$. Still, the effective mass of Eq. (4), relating velocity to momentum, exists, $m^*=E/u^2$. The equivalence between the energy and the mass, as given by Eq. (5), remains unchanged. An electron (hole) cannot be accelerated since its velocity is constant, $v=u$. It corresponds to $1/M^*=d^2E/dp^2=0$, i.e., to $M^*=\infty$. This indicates once again that the mass m^* is more useful than M^*. The above features describe "massless" electrons (holes) which acquire their mass due to motion. According to Eq. (9) the length of zitterbewegung is $\lambda_Z=\infty$. Using the initial Hamiltonian (1) with $a_n=0$ and the definition of the quantum velocity $\hat{v}$ it can be easily verified that $d\hat{v}/dt=0$. Thus, also the quantum velocity is constant, from which we conclude that in metallic CNT the carriers in the lowest subband do not experience the zitterbewegung.

The subject of zitterbewegung is lately very intensively discussed in the literature, see Refs. 26–29. It has been concluded that this phenomenon should occur in many situations in solids but no viable ways of its observation have been proposed.

V. SUMMARY

In summary, using the analogy between the band structure of single-wall semiconducting carbon nanotubes and the description of relativistic electrons in vacuum we formulate one-dimensional semirelativistic kinematics and dynamics for nonrelativistic charge carriers in CNT. We also consider the quantum domain demonstrating that electrons in CNT experience the zitterbewegung (trembling motion) even in absence of external fields. For typical diameters of CNT the amplitude of ZB should be of the order of nanometers. If the electrons are described by an effective one-band Hamiltonian for positive (or negative) energy, there is no ZB but the electrons should be treated as objects extended along the direction of the CNT axis. It is emphasized that the analogous effects have been predicted for relativistic electrons in vacuum but they are much more difficult to observe than in CNT.

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