Electron properties of Carbon nanotubes in the field effect regime

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Electron properties of Carbon nanotubes can change qualitatively in a transverse electric field. In metallic tubes the sign of Fermi velocity can be reversed in a sufficiently strong field, while in semiconducting tubes the effective mass can change sign. These changes in the spectrum manifest themselves in a breakup of the Fermi surface and in the energy gap suppression, respectively. The effect is controlled by the field inside the tube which is screened due to the polarization induced on the tube. The theory of screening links it with the chiral anomaly for 1D fermions and obtains a universal screening function determined solely by the Carbon π electron band.

The possibility to change electron spectrum of Carbon nanotubes by external field is of interest for basic research as well as for nanoscale device engineering. Carbon nanotube (NT) is a 1D metal or semiconductor depending on the chiral angle [1]. Metallic behavior can be suppressed by parallel magnetic field that induces a minigap at the band crossing [2]. Similar minigaps appear in nominally metallic chiral NTs due to the intrinsic curvature [3,4]. Novel properties are predicted for the BN tubes having no inversion symmetry [5].

Here we examine the changes induced in the NT electron spectrum by transverse electric field $E$ strong enough to mix different NT subbands:

$$eE R \simeq \Delta_0 \equiv \hbar v / R, \quad E \text{[MV/cm]} \simeq \frac{5.26}{R^2} \text{[nm$^2$]}, \quad (1)$$

where $R$ is the tube radius and $v$ is electron velocity. In such a field the effect on electron spectrum is dramatic: in metallic tubes the electron velocity $v = dE / dp$ can be reduced and even reverse the sign, causing Fermi surface breakup, while in semiconducting tubes the effective mass sign can change, which is accompanied by strong suppression of the excitation gap (Fig.1).

The NT electron system in this regime can be a host of intriguing many-body phenomena. The reduction of electron velocity in metallic tubes leads to an increase of the transverse field within the tube, since a uniformly charged cylinder is equipotential. Charging may affect the inner NT field indirectly via changing screening, but this effect should not be significant at moderate gating.

The π electron Carbon band is described by a nearest-neighbor tight-binding problem $e\psi_r = t \sum_{\nu} \psi_{r\nu}$ with the hopping amplitude $t \simeq 3 \text{eV}$. The states with small $|e| \ll t$ are described, separately at each of the $K$ and $K'$ points, by a massless Dirac Hamiltonian

$$H_0 = -i\hbar \nu (\sigma_y \partial_x - \sigma_x \partial_y), \quad v = 3ta_{c-c}/2\hbar \quad (2)$$

For a NT in the presence of a transverse electric field $E$,

$$H_0 = \hbar v (i\sigma_x \partial_y + \sigma_y k) - eE R \cos(y/R) \quad (3)$$

with $k$ the longitudinal momentum and $R$ the NT radius. The boundary conditions are quasiperiodic:

$$\psi(y + 2\pi R) = e^{2\pi i\delta} \psi(y), \quad \delta = \begin{cases} 0, & \text{metallic} \\ \pm \frac{1}{3}, & \text{semic.} \end{cases} \quad (4)$$
The effects of NT curvature as well as of a parallel magnetic field can in be included by slightly shifting \( \delta \) away from the ideal values.

We employ a chiral gauge transformation
\[
\psi(y) = e^{-i\sigma_x \phi(y)} \tilde{\psi}(y) , \quad \phi(y) = \frac{e \epsilon R^2}{\hbar v} \sin(y/R) \tag{5}
\]
which preserves the condition and turns Eq. (3) into
\[
\tilde{H}_0 = \hbar v \left( i \sigma_x \partial_y + k e^{2i\sigma_x \phi(y)} \sigma_y \right) \tag{6}
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Electron velocity changes sign at the roots of the Bessel function \( J_0 \), first at \( 2u = \mu_1 \approx 2.405 \) (Fig. 1). At \( u \) above critical the Fermi surface fractures: an additional small pocket appears for each spectral branch.

The level shifts in semiconducting NT at small \( k \) are given by the second order perturbation theory in the \( k \)-term of the transformed Hamiltonian (7):
\[
\epsilon_n^\pm(k) = \pm \Delta_0 \left( (n + \delta) + A_n(kR)^2 \right) \tag{8}
\]
\[
A_n = \sum_{m=-\infty}^{\infty} J_n^2(2u) \frac{2(n + \delta)}{4(n + \delta)^2 - m^2} \tag{9}
\]
For \( \delta = 1/3 \) the curvature of the lowest band \( A_0 \) changes sign at \( u_c \approx 0.6215 \) (Fig. 1). This leads to a singular behavior of the excitation gap which is constant at \( u < u_c \) and sharply decreases at \( u > u_c \) (Fig. 1 inset). This occurs because of the lowest excitation energy shifting from \( k = 0 \) at \( u < u_c \) to \( k \neq 0 \) at \( u > u_c \). The threshold-like suppression of the gap can be detected by a transport measurement in a thermally activated regime.

The chiral gauge symmetry (8) that protects the spectrum at \( k = 0 \) is a distinct feature of the Dirac model (4). The \( \pi \) electron tight-binding problem, in the next-lowest gradient order, generates a correction to the Hamiltonian (8) violating the symmetry (8):
\[
H = H_0 + \lambda e^{-i\theta \sigma_z} [\sigma_x (\partial_x^2 - \partial_y^2) - 2\sigma_y \partial_x \partial_y] e^{i\theta \sigma_z} \tag{10}
\]
with \( \lambda = \frac{8 - \delta}{8} e \hbar v \) and \( \theta \) the NT chiral angle (8). The transformation (8) applied to (10) gives a minigap (11)
\[
\Delta_{\epsilon} = | \sin \theta | (a_{\epsilon - \epsilon}/8\hbar v) (e \epsilon R)^2 \tag{11}
\]
Since \( 8R \gg a_{\epsilon - \epsilon} \), the minigap (11) is too small to alter the behavior at the energies of interest, \( \epsilon \approx \Delta_0 \).

The main effect of electron interaction is screening of the inner field that couples to the electron motion. Here we derive the relation between the inner and outer fields. We first show how the screening problem is reduced to the calculation of the NT electron energy in the presence of an external field. Hereafter we measure all energies in the units of \( \Delta_0 = \hbar v/R \) and use dimensionless field \( u = e \epsilon R/\Delta_0 \). From Gauss’ law, the fields inside and outside the tube are related with the induced surface charge density per one fermion species (spin and valley) by
\[
\epsilon_{\text{ext}} = \epsilon + \frac{1}{2} \cdot 4\pi \cdot 4 \sigma \tag{12}
\]
where the factor \( 1/2 \) accounts for depolarization in the cylindrical geometry. In Eq. (12) we projected the actual charge density on the \( \cos \varphi \) harmonic as \( \sigma(\varphi) \rightarrow 4\sigma \cos \varphi \), ignoring the higher order harmonics. (Here \( \varphi \equiv y/R \).)

To obtain the \( \cos \varphi \) harmonic of the induced charge, we evaluate the dipole moment per unit length as \( P = \)
$-dW(\mathcal{E})/d\mathcal{E}$, where $W(\mathcal{E})$ is the energy of one fermion species as a function of the inner field. Combining this with the relation $\sigma = P/(\pi R^2)$ and with the Gauss’ law \footnote{12}, and passing to dimensionless $u_{\text{ext}}$, $u$, we obtain

$$u_{\text{ext}} = u + \frac{e^2}{\hbar v} P(u)$$  \hspace{1cm} (13)

After the dipole moment $P(u)$ is known Eq.(13) can be solved for the inner field $u$ in terms of the outer field $u_{\text{ext}}$.

We consider the general problem of electron energy in a transverse field in a free particle model. The electron levels $\epsilon_{n,k}$ perturbed by the field can be easily found numerically at each value of the longitudinal momentum $k$ by using a transfer matrix for Eq.(13). The level shifts $\delta \epsilon_{n,k} = \epsilon_{n,k}(u) - \epsilon_{n,k}^0$ decrease at large $|n|$, and the series the total change of the occupied states energy

$$E_0(k) = \sum_{n = -\infty}^{+\infty} \delta \epsilon_{n,k} \quad \text{(such that } \epsilon_{n,k}(u) < 0)$$  \hspace{1cm} (14)

rapidly converge at $n \to \pm \infty$.

There are two basic problems with Eq.(14): 1) Due to an upward shift of the filled levels (Fig.1), $E_0$ is positive and also has positive derivative $dE_0/du$. Hence Eq.(14) leads to the dipole moment $P_0 = -dE_0/du$ opposite to the field, i.e. to an unmagnetic “diamagnetic” polarization sign instead of the expected “paramagnetic” effect. 2) The dependence of the energy $E_0$ on the longitudinal wavevector $k$ leads to an ultraviolet divergence in the integral $P = \int P(k)dk$, because $E_0(k)$ increases with $|k|$, saturating at $|k|R \gg 1$ at an asymptotic value $\frac{1}{2}u^2$.

Both difficulties are resolved by taking into account a fundamentally important contribution to the energy that arises due to the effects at the Fermi sea bottom. Physically, the finite electron band width invalidates the massless Dirac approximation at large negative energies. This contribution, however, depends solely on the number of Dirac fermion species and their velocity $v$, and is totally insensitive to any other details including the longitudinal momentum $k$ value. We find that

$$E_{\text{anom}} = -\frac{u^2}{2}$$  \hspace{1cm} (15)

for each fermion species. Remarkably, Eq.(15) can be obtained without detailed discussion of the behavior at the interatomic length scales — the universality of Eq.(15) is rooted in the physics of the chiral anomaly in the 1+1 fermion problem. The resulting total energy integral

$$W = \int_{-\infty}^{\infty} (E_0(k) + E_{\text{anom}}) \frac{dk}{2\pi}$$  \hspace{1cm} (16)

converges after $E_0(k)$ is offset by $E_{\text{anom}}$ (Fig.2).

We evaluate the energy \footnote{12} and derive the anomaly \footnote{13} for a weak field $u \ll 1$. The NT bands at $u = 0$ are

$$\epsilon_n^\pm(k) = \pm \sqrt{(n + \delta)^2 + k^2}, \quad -\infty < n < +\infty$$  \hspace{1cm} (17)

In a half-filled system with just the $\epsilon_n^-(k)<0$ bands filled, the external field $u$ changes the Fermi sea energy by

$$W = -\int \sum' \delta \epsilon_n^-(k) \frac{dk}{2\pi}$$  \hspace{1cm} (18)

Here the superscript in $\sum'$ indicates regularization by truncating the interaction with the external field at a certain large negative energy. We check that this contribution to the energy is independent of the details of truncation and obtain the anomaly \footnote{14} by choosing a convenient truncation scheme.

![FIG. 2. Dipole moment $P(k) = -d(E_0(k) + E_{\text{anom}})/du$ per one fermion species in a semiconducting NT as a function of $k$. Note that the energy anomaly \footnote{15} cancels with $E_0(k)$ at $kR \gg 1$, assuring convergence of $P_{\text{total}} = \int P(k)dk/2\pi$. Note also that $P(k \to 0)$ is dominated by the anomaly, since $E_0 = 0$ at $k = 0$ due to the chiral gauge invariance \footnote{15}.](image-url)

The level shifts $\delta \epsilon_n^-(k)$, in the second order of the perturbation theory in the external field $\tilde{V} = -e\mathcal{E}R \cos \varphi$, are

$$\delta \epsilon_n^- = \sum_m \frac{|\langle m^+|\hat{V}|n^-\rangle|^2}{\epsilon_n - \epsilon_m^+} + \sum_m \frac{|\langle m^-|\hat{V}|n^+\rangle|^2}{\epsilon_n - \epsilon_m^-}$$  \hspace{1cm} (19)

where the superscript $\pm$ indicates the electron and hole branches and the $k$ dependence is suppressed. Due to the integration over $\varphi$ with $V \propto \cos \varphi$ in the matrix elements the only nonzero terms in (19) are those with $m = n \pm 1$.

We now show that the sums over $\epsilon_m^-$ and $\epsilon_m^+$ in (19), respectively, give the regular and the anomalous contributions to the total energy $W = \sum' \delta \epsilon_n^-$. Different behavior of the two sums under regularization stems from their different convergence type. Individual terms in the sum over $\epsilon_m^-$ decrease rapidly at large $m$, so that the series for $W$ is absolutely convergent. On the other hand, in the sum over $\epsilon_m^+$ the terms do not change at large $m$ and thus the corresponding contribution to $W$ is given by poorly convergent and regularization-sensitive series.

Taking from (19) just the terms with $\epsilon_m^+$, evaluating the matrix elements $\langle m^+|\hat{V}|n^-\rangle$ and summing over $n$ yields

\footnote{15}
\[ E_0(k) = \frac{u^2}{4} \sum_n \frac{e_n^+(k) e_n^+(k) - (n+\delta)(n'+\delta) - k^2}{e_n^+(k) e_n^+(k)(e_n^+(k) - e_n^+(k))} \]  

(20)

with \( n' = n + 1 \). The sum \( (20) \) rapidly converges at large \( n \to \pm \infty \) and can be easily evaluated numerically.

Now we consider the sum of the level shifts \( W = \sum_n \delta e_n^- \) taking into account only the second term in \( (19) \). At the first sight this sum is identically zero. Indeed, due to the symmetry \( \langle n^-|\hat{V}|n^-\rangle = \langle n^-|\hat{V}|n^-\rangle \), in the sum over \( n \) with \( n = n \pm 1 \) all the terms cancel in pairs. However, truncation of the interaction at a large negative energy compromises the cancellation and yields a finite result. If one sets \( \langle m^-|\hat{V}|n^-\rangle = 0 \) for all \( |m| \text{ or } |n| \) exceeding a large number \( N \), there will be just two terms in the sum over \( n \) that do not cancel:

\[ E_{\text{anom}} = \frac{|\langle N'|-\hat{V}|N'\rangle|^2}{\epsilon_{N'} - \epsilon_{N'}} + \frac{|\langle -N'|-\hat{V}|N'\rangle|^2}{\epsilon_{-N'} - \epsilon_{-N'}} \]  

(21)

with \( N' = N - 1 \). Evaluating the matrix elements and energy levels is straightforward because at large \( N \gg |k| \) one can set \( k = 0 \). The result, coinciding with \( (15) \), is robust under a change of the regularization.

The expression \( (13) \) for the energy anomaly, derived above for the weak field, is in fact more general. To illustrate this we consider a special case of zero longitudinal momentum \( k = 0 \) and derive \( (13) \) from bosonization, without using perturbation theory in \( u \ll 1 \). After the problem \( (7) \) is bosonized in the standard way \( [12] \), using \( \psi_{L,R} \propto e^{i\phi_L}, e^{-i\phi_R} \), we obtain a quadratic Hamiltonian

\[ \mathcal{H} = \int_0^{2\pi R} \sum_{j=L,R} \left[ \frac{\mu}{\pi} (\partial_\phi \phi_j)^2 + \frac{\epsilon}{\pi} \partial_\phi \phi_j U(y) \right] dy \]  

(22)

The second term in \( (22) \) representing interaction with the external field \( U(y) \) can be decoupled by a shift \( \phi_j \rightarrow \phi_j' - \frac{1}{\partial U/\partial y} \int_0^y U(y')dy' \). The Hamiltonian for \( \phi_j' \) takes the form \( (23) \) with \( U = 0 \), while the ground state energy

\[ \delta E = -\frac{e^2}{2\pi \hbar v_F} \int_0^{2\pi R} U^2(y) dy \]  

(23)

is nothing but the anomaly \( (15) \) scaled by \( \Delta_0 = \hbar v/R \).

After adding the energies \( (20) \) and \( (15) \), and integrating in \( (14) \) over \( k \), one obtains

\[ W = -\frac{\alpha}{2} u^2, \quad \alpha = \left\{ \begin{array}{ll} 0.196... & \text{for } \delta = 1/3 \\ 0.179... & \text{for } \delta = 0 \end{array} \right. \]  

(24)

Eq. \( (12) \) with the dipole moment \( P = -dW/dE \) and the charge density \( \sigma = P/\pi R^2 \) yield the screening function

\[ \mathcal{E}_{\text{ext}} = \left( 1 + 8\alpha \frac{e^2}{\hbar v} \right) \mathcal{E} \]  

(25)

With \( e^2/\hbar v = 2.7 \) this gives \( \mathcal{E}_{\text{ext}}/\mathcal{E} = 5.24 \) for \( \delta = 1/3 \), and \( \mathcal{E}_{\text{ext}}/\mathcal{E} = 4.87 \) for \( \delta = 0 \). The outer-to-inner field ratio \( \zeta \approx 5 \) (see \( (10) \) for another derivation) renders the required fields \( (7) \) feasible \( [3] \). Interestingly, the screening \( (25) \) is independent of the tube radius \( R \) and is almost the same in the metallic and semiconducting NTs. The latter is not surprising, since the screening is absent in a single 1D mode approximation: the polarizability is related with dipolar transitions between different subbands.

The radius-independence of \( (27) \) resembles an effect of a dielectric constant. We note, however, that the change of the inner field due to individual Carbon atoms polarizability is small in \( a_{c-c}/2\pi R \ll 1 \). The result \( (24) \) reflects the semimetallic character of the \( \pi \) electron band with the density of states vanishing at the band center.

In summary, nanotube electron states undergo interesting transformations in the field effect regime, leading to novel phenomena in both the single particle and many-body properties. The analysis of screening, performed using a relation with the theory of chiral anomaly, indicates that the fields required for the observation of the proposed effects are in the experimentally feasible range.

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