Energy Anomaly and Polarizability of Carbon Nanotubes

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The energy of electron Fermi sea perturbed by external potential, represented as energy anomaly which accounts for the contribution of the deep-lying states, is analyzed for massive $d = 1 + 1$ Dirac fermions on a circle. The anomaly is a universal function of the applied field, and is related to known field-theoretic anomalies. We express transverse polarizability of Carbon nanotubes via the anomaly, in a way which exhibits the universality and scale-invariance of the response dominated by $\pi$ electrons and qualitatively different from that of dielectric and conducting shells. Electron band transformation in a strong-field effect regime is predicted.

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Fermion anomalies are universal contributions to low-energy properties of field theory originating from the bottom of the filled Fermi-Dirac sea. The primary examples in high-energy physics are the spontaneously generated photon mass in $d = 1 + 1$ \cite{a}, and the Adler-Bell-Jackiw chiral anomaly \cite{b} relating the decay of pion into two photons to the number of quark colors \cite{c}. Several instances of anomalies are known in solid state physics, with the chiral anomaly manifest in transport \cite{d} and in fermion number fractionalization \cite{e}, and the parity anomaly in $d = 2 + 1$ linked to the quantum Hall effect \cite{f}.

Here we describe a new manifestation of fermion anomaly, appearing in the total energy of Fermi sea in the presence of an external field. While the net energy of Fermi-Dirac vacuum depends on ultraviolet cutoff, i.e. on the behavior at the bottom of the band, we find the external field-dependent part of the energy to be cutoff-insensitive. The latter energy is naturally divided into two parts, one given by a sum of the energy shifts of filled states near the Fermi level, and another, equally important, describing cumulative effect of the states deep below the Fermi level. The latter, anomalous part, traced to Schwinger anomaly \cite{g}, has a universal form and can be expressed through the properties near the Fermi level.

The Fermi sea energy field-dependence is the physical quantity central for many physical properties of materials. As an application, below we consider the response of the carbon nanotube (NT) $\pi$ electron band to perpendicular electric field. The aforementioned separation into the normal and anomalous parts enables one to handle energy in a fully general and, at the same time, case-specific way, taking full account of the level quantization, curved geometry, spatial inhomogeneity, etc. The NT $\pi$-band is described by a tight-binding model on a honeycomb lattice \cite{h}. Near the Fermi level, at the $\pi$-band center, the NT electrons are described by $2 + 1$ Dirac fermions moving on a cylindrical surface \cite{i}. Dirac model provides a simple analytic description of NT curvature and chirality \cite{j,k}, and of the effects of external fields \cite{l} in both semiconducting and metallic NTs.

It might seem that understanding properties such as NT polarizability should require a detailed knowledge of the $\pi$ electrons behavior on the lattice constant scale \cite{m}. Here we find that, to the contrary, the energy calculated from Dirac model, with the anomaly properly accounted for, not only is numerically accurate, but also provides new insight into NT properties. We identify the dominant role of $\pi$ electrons response compared to that of other orbitals, and explain the origin of the scale-invariant depolarization, independent of the NT diameter \cite{n,o,p}, qualitatively different from that of metallic and dielectric shells. Our approach, with electron interactions included in an RPA fashion \cite{q}, is not limited to linear response: we apply it to study NT electron band transformation in the field-effect regime.

The origin of the energy anomaly is exhibited most clearly by the example of chiral 1d fermions on a circle $[0, 2\pi]$, described by the Hamiltonian $\mathcal{H} = -i\partial_{\theta} + U$, $U = 2a \cos \theta$. In the Fourier representation $|n\rangle = e^{in\theta}$, $\mathcal{H}$ is given by an infinite three-diagonal matrix: $\mathcal{H}_{nn} = n$, $\mathcal{H}_{n\pm 1} = a$. Eliminating the potential $U$ by a gauge transformation $\psi(\theta) = e^{-2ia \sin \theta} \psi(\theta)$, $\mathcal{H} = -i\partial_{\theta}$, we see that the eigenvalues of $\mathcal{H}$ are integers independent of $U$.

The energy anomaly arises when the interaction $U$ is truncated at a certain energy scale. To that end, let us consider a more general three-diagonal matrix

$$\mathcal{H}_{nn} = n, \quad \mathcal{H}_{n+1,n} = \mathcal{H}_{n+1,n} = a_n, \quad n \in \mathbb{Z},$$

with the sequence $a_n$ having different limits at $n \to \pm \infty$: $a_{n \to -\infty} = 0$, $a_{n \to +\infty} = a$. Although now the energy levels depend on $a_n$, the above argument for spectrum robustness at constant $a_n$ indicates that this dependence is exponentially small at large $|n|$. The level shifts are significant only for a relatively small cluster of levels around $n \approx n_a$ where the switching of $a_n$ from 0 to $a$ occurs.

Notably, the sum of all level shifts, $\delta tr \mathcal{H} = \sum_n \delta \epsilon_n$, depends only on the asymptotic values $a_{n \to \pm\infty}$, while other details of the sequence $a_n$ do not matter. To see this, we truncate the matrix $\mathcal{H}$ at some large positive and negative $n = \pm N$, in which case the trace of this
(2N + 1) \times (2N + 1) \text{ matrix is finite and explicitly } a\text{-independent. Since at } N \gg n_*, \text{ the mutual influence of the levels at } n \approx n_* \text{ and } n \approx N \text{ is exponentially small, the effect on } \text{tr } \mathcal{H} \text{ due to truncating at } n \approx N \text{ is negative of that due to } a_n \text{ switching at } n \approx n_*, \text{ both being universal. [The levels at } n \approx -N \text{ are unaffected by the truncation since } a_{n \rightarrow -\infty} = 0 \text{ and } \mathcal{H} \text{ is diagonal.] Thus the sum of the level shifts at } n \approx n_* \text{ depends only on } a_{n=+\infty} = a, \text{ giving a cutoff-independent contribution to } \delta \text{tr } \mathcal{H}.

The universal value \( E_{\text{anom}} = \delta \text{tr } \mathcal{H} \) can be evaluated using slowly varying \( a_n, \{da_n/da\} \ll |a_n| \). In this case, since the levels are unperturbed by constant \( a_n \), the level shifts will be small, which warrants using perturbation theory. Gradient expansion of \( a_n \) in the vicinity of \( n = n_* \) yields \( \mathcal{H} = -i\partial_y + 2a \cos \theta + b \{ e^{i\theta} (-i\partial_y) + \text{h.c.} \} \), with \( a = a_n - bn_*, b = da_n/\{dn|n=n_*=a \). The gauge transformation \( \psi(\theta) = e^{-2a \sin \theta \psi(\theta)} \) transforms \( \mathcal{H} \) into

\[
\tilde{\mathcal{H}} = -i\partial_y + b \{ e^{i\theta} (-i\partial_y - 2a \cos \theta) + \text{h.c.} \} \tag{2}
\]

The energies \( \epsilon_n \) with \( n \) near \( n_* \) obtained in the lowest order of perturbation theory are \( \epsilon_n = (n|\tilde{\mathcal{H}}|n = n - 2a_n \). The sum of these level shifts, given by a full derivative, depends only on the asymptotic of \( a_n \):

\[
E_{\text{anom}} = -\sum_n 2a_n \approx -\int_{-\infty}^{\infty} dn 2a_n \frac{da_n}{dn} = -a^2. \tag{3}
\]

The relation of this result with fermionic energy emerges when one considers quantization of the external field \( a_n = a \) coupling to the states at the Fermi sea bottom, modeled by \( a_{n \leq n_*} = 0 \). We find that the anomalous contribution \( E_{\text{anom}} \) is universal, i.e. it depends only on the properties near Fermi level \( \mathcal{E}_F \). The anomaly contributes additively to the energy along with the contributions due to fermion mass and confinement (see below).

Electrons in a nanotube, a cylinder of radius \( R \), are described by \( 2 + 1 \) massless Dirac model \( \mathcal{H}_D \). The states in a transverse field, labelled by momentum \( k \) along the tube, can be viewed as massive \( 1 + 1 \) Dirac fermions on NT circumference, the circle \( 0 < y < 2\pi R \):

\[
\mathcal{H}_D = -i\hbar v \hat{a} \partial_y + \hbar vk \hat{\beta} + U(y), \tag{4}
\]

with \( U(y) \) the transverse field potential and \( \hbar vk \) the Dirac “mass”. (Here \( \hat{\alpha} = -\sigma_x \) and \( \hat{\beta} = \sigma_y \).) We assume generic quasiperiodic boundary conditions \( \psi(y + 2\pi R) = e^{2\pi i \delta} \psi(y) \). At \( U \equiv 0 \), the energy levels

\[
\epsilon_n^\pm = \pm \sqrt{\Delta^2_R (n + \delta)^2 + (\hbar vk)^2}, \quad \Delta_R \equiv \hbar v / R, \tag{5}
\]

describe NT minibands. The phase \( \delta \) determines NT properties: \( \delta = \frac{1}{4} \) for semiconducting NT, \( \delta = 0 \) for metallic NT, and \( |\delta| < 1 \) for the tubes with small gap induced by curvature \( \mathcal{K} \) or by parallel magnetic field \( B \).

For the Fermi sea energy at finite \( U \), the naive answer would be the sum over occupied states \( W = \sum \delta \epsilon_n \)

\[
\delta \epsilon_n = \epsilon_n |U| - \epsilon_n |U=0| . \tag{6}
\]

The level shifts \( \delta \epsilon_n \) become very small away from the band center, at \( |n| \gg kR \). In this limit, with the contribution of finite mass being negligible, the Dirac problem decouples into two chiral fermion modes, each having \( U \)-independent spectrum. However, despite the absence of level shifts, the states with large \( n \) contribute to the \( U \)-dependent energy via anomaly due to the bandwidth cutoff, \( (\hbar v / R)n_\sim \sim -10eV \) for Carbon. As described above, the anomaly depends only on the properties near the band center:

\[
E_{\text{anom}} = -\frac{N_f}{2\pi \hbar v} \int_0^{2\pi R} U^2(y)dy, \tag{7}
\]

where \( N_f = 4 \) is the number of electron flavors associated with spin and the points \( K, K' \). Note that the energy \( \mathcal{E}_F \) is additive for multiple fermion flavors, contrary to fermion-doubling cancellation typical of the chiral anomaly effects \( \mathcal{E}_F \).

One can interpret Eq. (4), somewhat loosely, as a counterterm which eliminates the nonphysical contribution of infinite Fermi sea in the model \( \mathcal{H}_D \), i.e. the states outside the Carbon band. A photon mass \( m_\gamma^2 = e^2 / \pi \) appears in \( d = 1 + 1 \) QED \( \mathcal{E}_F \) after integration over massless fermions. Eq. (4) exhibits a similar effect in the Dirac system in an external electromagnetic field \( eA_{\mu} = (U(y), 0) \), with the mass term \( \int d^2 x \frac{1}{2} m_\gamma^2 A_{\mu} \equiv -\int E_{\text{anom}} dt \) in the action. [We point out a distinction of our approach and Coleman’s analysis \( \mathcal{E}_F \) of massive Schwinger model in external field, which yields an effective action containing the field intensity rather than potential.]

The energy anomaly is related to the chiral anomaly in \( d = 1 + 1 \), since in this case the chirality \( \gamma^5 \) enters the Hamiltonian \( \mathcal{H}_D \). Formally this can be seen via the change in the functional measure \( \mathcal{E}_F \). First note that a chiral gauge transformation \( \mathcal{H} \rightarrow \mathcal{H}' = e^{-i\gamma^5 \phi \tilde{\psi}} \tilde{\psi}, \quad \phi = \int dy U(y)', \tag{8}
\]

preserves the boundary conditions \( \psi \), turning \( \mathcal{H}_D \) into

\[
\tilde{\mathcal{H}}_{D} = -i\hat{a} \partial_y + k e^{2i\gamma^5 \phi \tilde{\psi}} \tilde{\psi}. \tag{9}
\]

Consider now the variation of the background field \( U(y) \) by \( \delta U(y) \), related to the infinitesimal transformation \( \mathcal{E}_F \), \( \psi' = e^{i\gamma^5 \phi(y)} \tilde{\psi}, \lambda(y) = \int dy \delta U(y) \). The corresponding Jacobian \( J = \exp(2i \int dy dy' \lambda(y')) \) changes the action by \( -i \ln J = -\delta E_{\text{anom}} \), yielding \( \delta E_{\text{anom}} = \frac{1}{2} \int dy \lambda \partial_y U, \text{ with } \lambda = \text{tr } \gamma^5 = \frac{1}{2i} e^{iU} F_{\mu\nu} = -\partial_y U(y') / 2\pi \) the 2d anomaly \( \mathcal{E}_F \). Integration by parts gives the variation \( \delta E_{\text{anom}} = -\frac{1}{2} \int dy \partial_y U \partial U, \text{ which is equivalent to the result \( \mathcal{E}_F \) [20]. This derivation can be extended to include electron interactions, proving robustness of the anomaly.}

Turning to the NT response to transverse electric field,

\[
U(y) = -eER \cos(y / R), \tag{10}
\]
we relate polarizability to the sum of Stark shifts

$$E_0(k) = \sum_{n=-\infty}^{+\infty} \delta \epsilon_n(k)$$

$$\delta \epsilon_n(k) = \epsilon_n(k) - \epsilon_n(k)|\epsilon=0,$$

taken over all occupied states, with $k$ the electron momentum along the tube. We obtain the shifts $\delta \epsilon_n(k)$ from the Hamiltonian \(\ref{eq:Hamiltonian}\). In this calculation, the anomaly \(\ref{eq:anomaly}\) must be added to account for the finite band cutoff, formally absent in \(\ref{eq:Hamiltonian}\).

The main effect of electron interaction is depolarization, i.e. screening of the field inside NT. To obtain the RPA screening function \(\ref{eq:screening}\) of NT cylinder, we first show how the problem is reduced to the calculation of electron energy in the presence of an external field. The Gauss’s law relates the fields inside and outside the tube with the induced surface charge density $\sigma$.

$$\mathcal{E}_{\text{ext}} = \mathcal{E} + \frac{1}{2} \cdot 4\pi \cdot N_f \sigma, \quad \sigma = \mathcal{P}/(\pi R^2),$$

where $\mathcal{P}$ is the dipole moment per flavor and per unit NT length, and the factor $1/2$ accounts for depolarization in cylindrical geometry. In Eq. \(\ref{eq:screening}\) we projected the actual charge density on the $\cos \varphi$ harmonic, $\varphi = y/R$, as $\sigma (\varphi) \rightarrow N_f \sigma \cos \varphi$, ignoring higher order harmonics.

The problem is then reduced to evaluating the dipole moment, given by $\mathcal{P} = -dW(\mathcal{E})/d\mathcal{E}$, where $W(\mathcal{E})$ is one fermion flavor energy as a function of the inner field,

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

Combining this with Eq. \(\ref{eq:screening}\), and using dimensionless $u = e\mathcal{E}R/\Delta R$, we obtain $u_{\text{ext}} = u + 2N_f \frac{\pi^2}{\hbar^2} \mathcal{P}(u)$. Once the dipole moment $\mathcal{P}(u)$ is known, this relation determines the inner field $u$ in terms of the outer field $u_{\text{ext}}$.

Taking the Stark shifts $\delta \epsilon_n(k)$ to the lowest order in $\mathcal{E}$ and evaluating the integral over $k$ (see Fig\(\ref{fig:diagram}\)), we obtain

$$W = -\frac{\alpha}{2} u^2, \quad \alpha \approx \begin{cases} 0.196... \text{ for } \delta = 1/3, \\ 0.179... \text{ for } \delta = 0. \end{cases}$$

Notably, the linear relation $\mathcal{P} = \alpha u$ holds up to very large fields $u \sim 1$ (Fig\(\ref{fig:diagram}\) inset), giving the depolarization

$$\mathcal{E}_{\text{ext}} = \left(1 + 2N_f \alpha \frac{\mathcal{E}}{\hbar^2} \right) \mathcal{E}.$$  

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 $\delta = 0$, in excellent agreement with the full tight-binding calculations \(\ref{eq:screening}\).

The screening \(\ref{eq:screening}\) is radius-independent and is nearly the same in the metallic and semiconducting NTs. The latter is not surprising: screening is absent in a single 1d mode approximation, sicne polarizability is related to dipolar transitions between different subbands. The scale-invariance of \(\ref{eq:screening}\) obtained for a hollow NT cylinder resembles depolarization in a massive dielectric cylinder.

FIG. 1: Partial dipole moment $P(k) = -d(E_0(k)+E_{\text{anom}})/du$ as a function of $k$, obtained from \(\ref{eq:screening}\) for semiconducting NT, where $u = e\mathcal{E}R/\hbar v$ is dimensionless field. Note the cancellation between $E_0(k)$ and the anomaly \(\ref{eq:anomaly}\) at $kR \gg 1$, enforcing convergence of $\mathcal{P} = \int P(k)dk/2\pi$. Note also that $P(k \rightarrow 0)$ is dominated by the anomaly, since $E_0 = 0$ at $k = 0$ due to the chiral gauge invariance \(\ref{eq:anomaly}\). Inset: Dipole moment $P$ on per fermion flavor versus $u$ for metallic and semiconducting NT. Straight lines represent weak field linearization \(\ref{eq:linearization}\). Arrow marks $u \approx 1.2$ for which velocity changes sign in metallic NT (see text and Fig\(\ref{fig:diagram}\)).

The dipole moment of $\pi$ electrons, found to scale with $R^2$, should be contrasted to $\mathcal{P} \propto R$ for hollow dielectric shell. The universal scale-invariant result \(\ref{eq:screening}\) reflects the dominant role of $\pi$ electrons in transverse response as compared to other Carbon orbitals.

To emphasize the role of anomaly in this calculation we note that omitting this contribution would have led to a wrong sign of the response and also to a divergence. Indeed, due to an upward shift of the filled levels $\epsilon_n$ (Fig\(\ref{fig:diagram}\)), we have $\mathcal{P}_0 = dE_0/du > 0$, corresponding to unphysical “diamagnetic” polarization sign. Also, the $k$-dependence $E_0(k)$ causes an ultraviolet divergence in the integral $\mathcal{P} = \int P(k)dk/2\pi$, since $E_0(k)$ 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 the negative $E_{\text{anom}} = -\frac{1}{2}u^2$. The resulting integral \(\ref{eq:screening}\) converges after $E_0(k)$ is offset by $E_{\text{anom}}$ (Fig\(\ref{fig:diagram}\)).

To illustrate the effect of transverse field, here we examine the NT electron spectrum. The changes are most dramatic in a strong field \(\ref{eq:field}\) which mixes different NT subbands, $u \approx 1$, or $e\mathcal{E}R \approx \Delta R$, $\mathcal{E} [\text{MV/cm}] \approx 5.26/R^2 [\text{nm}^2]$. In metallic NTs the electron velocity $v = de/dp$ decreases and can even reverse sign, causing Fermi surface breakup. This could lead to interesting many-body effects such as the Luttinger correlations increase due to enhanced $e^2/\hbar v$, or instability with respect to exciton formation for the negative-$v$ states. Semiconducting NTs exhibit the effective mass sign change, ac-


Metallic NT occurs at $u > u_c$.

Effects in semiconducting NT at

In summary, we considered the energy of Fermi sea $\varepsilon(k)$ in the units of $\Delta$, where $\varepsilon(k)$ is the energy of the fermions in the $k$-space.

The above screening calculation provides an estimate for the relative importance of the screening in semiconducting and metallic NT, and relative importance of the $\pi$ band compared to other Carbon bands. Electron bands exhibit dramatic change in the strong field-effect regime.

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