Fine structure of the local pseudogap and Fano effect for superconducting electrons near a zigzag graphene edge

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Motivated by recent scanning tunneling experiments on zigzag-terminated graphene this paper investigates an interplay of evanescent and extended quasiparticle states in the local density of states (LDOS) near a zigzag edge using the Green’s function of the Dirac equation. A model system is considered where the local electronic structure near the edge influences transport of both normal and superconducting electrons via a Fano resonance. In particular, the temperature enhancement of the critical Josephson current and $0 - \pi$ transitions are predicted.

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Introduction.- Experimental evidence\cite{1,2} for massless Dirac-like quasiparticles in graphene - a carbon monolayer with the hexagonal structure - has stimulated vigorous interest in electronic properties of this system (e.g. Refs. 3-11). The unit cell of graphene contains two atoms each belonging to a triangular sublattice, and the low-energy states are described by a two-dimensional Dirac equation where the role of spin is assumed by the sublattice degree of freedom (pseudospin)\cite{12,13}. Similar to relativistic spin-half particles in two dimensions, the graphene bulk density of states has a linear pseudospin\cite{14} around zero energy $E = 0$. Natural boundaries can however give rise to additional spectral branches such as the low-energy edge states\cite{14,15}. They are localized near a zigzag-shaped edge, whose outermost sites all belong to the same sublattice [Fig. 1(a)], and originate from the effective pseudospin "polarization" due to vanishing of one of the pseudospinor components as required by particle conservation\cite{14}. Recent scanning tunneling experiments\cite{16,17} report a singular enhancement of the LDOS near zigzag boundaries attributed to the edge states.

The measurements\cite{16,17} also revealed another peculiarity of the energy dependence of the LDOS - a fine oscillatory structure superimposed on the pseudogap with the amplitude enhanced at larger energies\cite{17}. The origin of this behavior is still unaccounted for, although subsequent publications have studied the graphene LDOS, e.g. numerical simulations of Ref. 18 found damped spatial oscillations of the LDOS. The present study intends to show that both findings are consistent with the picture of interfering Dirac electron waves near a zigzag edge. To demonstrate this point, the one-particle Green’s function of the Dirac equation was calculated for clean graphene with a zigzag edge described by the boundary condition of Ref. 5. Then, the following expression for the LDOS $\nu(E, d)$, as a function of energy $E$ and distance $d$ from the edge, was obtained

$$\nu(E, d) = |E| \frac{1 + J_0 \left( \frac{2Ed}{\hbar \nu} \right)}{\pi \left( \frac{2Ed}{\hbar \nu} \right)^2} - \frac{J_1 \left( \frac{2Ed}{\hbar \nu} \right)}{4\pi \hbar \nu d^2} + \delta(E) \frac{\pi \hbar}{4\pi \hbar d^2}. \quad (1)$$

Here the delta-functional term results from the dispersionless zero-energy edge state whereas the oscillating components given by the Bessel functions $J_0(2Ed/\hbar \nu)$ and $J_1(2Ed/\hbar \nu)$ are due to interfering waves formed of the states belonging to the Dirac spectrum ($v$ and $\hbar$ are the electron velocity and Planck’s constant). For $2Ed/\hbar \nu \gg 1$ the amplitude of the oscillations is proportional to $\sqrt{|E|/d}$ [see also Figs. 1(b) and (c)], which qualitatively agrees with both the experiment\cite{17} and numerical simulations\cite{18}.

Another issue this study focuses on is the connection between the local electronic structure of zigzag-terminated graphene and Fano scattering\cite{19}. Unlike earlier works [e.g. Ref. 20] where the Fano effect was due to resonant flux states in finite-size ribbons, here the Fano resonance is studied in a nanowire side-coupled to half-

FIG. 1: (Color online) (a) Schematic view of a zigzag graphene ribbon terminated by atomic lines belonging to different sublattices, conventionally denoted as A and B. (b) LDOS vs. energy at different distances from the edge: (A) $d = 4a$, (B) $d = 10a$, (C) $d = 50a$, (D) $d = 1000a$; where $a = 0.246$ nm is graphene’s lattice constant, $\nu_a = \pi \hbar / 2a$, and $E_a = \hbar / 2a$. (c) LDOS vs. distance from the edge for different energies: (A) $E = 0.15E_a$, (B) $E = 0.3E_a$, (C) $E = 0.5E_a$. The delta function in Eq. 1 is approximated by a Lorentzian $\alpha / (\pi (E^2 + \alpha^2))$ with $\alpha = 0.03E_a$. 

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Fourier components are $G$ and $\sigma$, transitions similar to those in ferromagnetic Josephson junctions. In the context of the Josephson effect in graphene nanostuctures, these issues have not yet been addressed.

**Green's function of a zigzag ribbon.**—Assuming no scattering between the two valleys, $K$ and $K'$, of graphene's Brillouin zone, one only needs to calculate the Green's function in one of them, e.g., $K$, where the Dirac equation reads $[\sigma_0 E + i\hbar v(\sigma_x \partial_x + \sigma_y \partial_y)]G = \sigma_0 \delta(x - x') \delta(y - y')$. Here the (retarded) Green's function $G_{ik|x,y}$, of $\sigma_0$ scattering between the two valleys, $K$ and $K'$, Pauli $\sigma_0$, and unity $\sigma_0$ matrices all act in pseudospin space. It suffices to solve the pair of equations for $G_{AA}$ and $G_{BA}$.

After expanding in plane waves $e^{ikx}$, the equations for the Fourier components are $G_{BA|ik} = (\hbar/v)(k + \partial_y)G_{AA|ik}$ and $[\partial^2_y q^2]G_{AA|ik} = (E/2\hbar^2 v^2)\delta(y - y')$ with $q^2 = k^2 - (E/hv)^2$. The solution can be sought in the form $G_{AA|ik}(y, y') = a(y')e^{-qy} + b(y')e^{qy} - Ee^{-qy} - Ee^{qy}/2\hbar^2 v^2 q$, where the last term is the Green's function of an unbounded system, and the coefficients $a(y')$ and $b(y')$ are to be found from the boundary conditions $B_{BA|ik}|_{y = 0} = (k + \partial_y)G_{AA}|_{y = 0} = 0$ and $G_{AA}|_{y = w} = 0$. This yields the following result

$$G_{AA|ik}(y, y') = E/2\hbar^2 v^2 Q \times$$

$$\times \left\{ \frac{k[\cosh q(w - |y - y'|) - \cosh q(w - y - y')]}{q \cosh qw - k \sinh qw} - \frac{q[\sinh q(w - |y - y'|) + \sinh q(w - y - y')]}{q \cosh qw - k \sinh qw} \right\}. \quad (2)$$

The poles of $G_{AA|ik}$, given by the equation $q = k \tanh qw$ (cf. Ref. 5), determine the excitation spectrum. As known\textsuperscript{12,13}, it has an almost flat branch merging with the Fermi level $E = 0$ corresponding to a state exponentially decaying from the edge into the interior. This can be easily seen from Eq. (2) in the limit $w \to \infty$:

$$G_{AA|ik}(y, y') = \frac{Ee^{-qy}}{2\hbar^2 v^2 q} + \frac{(q + k)e^{-q(y + y')}}{2qE}. \quad (3)$$

The pole $E = 0$ describes a dispersionless edge state existing for $k > 0$. From Eq. (3), an exact position representation for the Green's function $G_{AA}(x, y, y') = \int_{-\infty}^{\infty} dk G_{AA|ik}(y, y')/2\pi$ can be obtained as

$$G_{AA}(x, y, y') = \frac{EY_0(kE[|y - y'|] - iE|J_0(kE[|y - y'|])}{(2\hbar v)^2}$$

$$+ \frac{2EY_1(kE[|y + y'|] - iE|J_1(kE[|y + y'|])}{(2\hbar v)^2 k_E(y + y')}, \quad (4)$$

where $J_n(z)$ and $Y_n(z)$ $(n = 0, 1)$ are, respectively, the Bessel and Neumann functions, and $k_E = \sqrt{E^2/\hbar v}. The LDOS $G_{AA}(x, 0) \approx 1/4\pi Ew^2$ with $d_e \sim a$.

**Fano scattering off a zigzag edge.**—The behavior of the Green's function near the edge can have a direct impact on charge transport. Let us consider a quasi-one-dimensional wire (with conventional quasiparticle spectrum) coupled in parallel to a zigzag graphene edge via a small momenta. This yields

$$G_{AA}(x, y, y') \approx 1/\pi E(y + y')^2, \quad y, y' \to 0, \quad (5)$$

independent of material parameters. To regulate the divergence at $y = y' = 0$, due to the effective continuum description, it is convenient to introduce the cutoff $G_{AA}(x, 0) \approx 1/4\pi Ew^2$ with $d_e \sim a$.

**FIG. 2:** (a) Schematic view of a zigzag-edge graphene ribbon with a side tunnel contact to a nanowire connecting electron reservoirs 1 and 2. The contact is assumed point-like, i.e. its size is much bigger than the interatomic distances, but smaller than the electronic mean free paths in both wire and graphene. (b) Zero-temperature conductance $g$ (in units of $e^2/\hbar v$) vs. bias voltage $V$ for spin-degenerate $(h = 0)$ and spin-split $(h = 3\Gamma)$ edge state in graphene.
the zero-temperature Landauer conductance

Figure 2(b) shows the voltage dependence of

Matsubara frequencies

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fer between the superconductors. Since both electron
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son coupling is maintained due to the Andreev process
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E
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effect discussed earlier

Fano-like transmission antiresonance at E = 0 manifests complete
backscattering of an electron wave incoming from one of
the reservoirs. It is due to destructive interference be-
tween the electron wave directly transmitted through the
wire (without tunneling) and the wave transmitted via
tunneling through the graphene edge state whose energy
is pinned to the Fermi level in the wire. It is straightforward
to generalize the analysis to a spin-split edge state with energies \( \pm \hbar \) for spin projections \( \alpha = \pm 1/2 \). In this case, we have

\[
t_{\alpha}(E) = e^{i k_0 L} (E + 2 \alpha \hbar)/(E + 2 \alpha \hbar + i \Gamma).
\] (7)

Figure 2(b) shows the voltage dependence of the zero-temperature Landauer conductance
g(V) = e^2/(2\pi\hbar) \sum_{n=\pm 1/2} t_{\alpha}(E)(v)^2. For h \neq 0 the conductance dip is split due to the spin-filtering
effect discussed earlier \[44,45 \] in the context of possible applications in spintronics \[36 \].

Fano effect in a Josephson junction.- Let us fin-
discuss the case of superconducting reservoirs sup-
porting an equilibrium Josephson current. The Joseph-
sion coupling is maintained due to the Andreev process \[17 \] whereby an electron is retro-reflected as a Fermi-sea hole from one of the superconductors with the subsequent
hole-to-electron conversion in the other one. Such an
Andreev reflection circle facilitates a Cooper pair trans-
fer between the superconductors. Since both electron
and hole also experience normal scattering inside the
junction, the transmission antiresonance is expected to
strongly influence the Josephson current. It is conve-
ient to use the approach of Refs. \[38,39 \] relating the su-
current to the scattering amplitudes via a sum over the
Matsubara frequencies \( \omega_n = (2n+1)\pi k_B T \) as follows

\[
I_c = -4e k_B T/h \sum_{n \geq 0, \alpha} a_{\alpha}^2(E) t_{\alpha}(E) t^*_{\alpha}(-E)|E=\omega_n, \] (8)

where \( t^*_{\alpha}(-E) \) is the hole transmission amplitude cor-
responding to the time-reversed counterpart of the elec-
tron Hamiltonian \[38,40 \], and \( a_{\alpha}(E) \) is the Andreev reflec-
tion amplitude at the point contacts to superconductors
in superconductors \[42,43 \], respectively. In this case the Joseph-
son-phase relation is sinusoidal with \( I_c[Eq. (8)] \) being the critical value of the current.

In contacts to conventional Bardeen-Cooper-Schrieffer
(BSC) superconductors, the Andreev process is well
described by the scattering model of Ref. \[44 \]. How-
ever, in many practical cases superconducting contacts
to low-dimensional systems can hardly be regarded as
BCS-like ones. Proximity-effect contacts to semiconduc-
tor nanowires \[44,45 \] and carbon nanotubes \[44,45 \] are impor-
tant examples of such a situation. In this case a thin
normal-metal layer is inserted between the superconduc-
tor and the wire to ensure a good electrical contact.
In proximity-effect point contacts the Andreev scatter-
ing amplitude can be expressed in terms of the qua-
sicalclassical condensate \( F_{\alpha}(\omega_n) \) and quasiparticle \( G_{\alpha}(\omega_n) \)
Green’s functions of the normal layer as \[40,47 \] \( a_{\alpha}(\omega_n) = i F_{\alpha}/(1 + G_{\alpha}) \). I will adopt this approach and make use of McMillan’s expressions \[48,49 \] for the Green’s func-
tions: \( F_{\alpha} = \Delta_n/\sqrt{\Delta_n^2 + \alpha^2} \), \( G_{\alpha} = (\omega_n/\Delta_n) F_{\alpha} \), and \( \Delta_n = \gamma \Delta/\sqrt{\gamma^2 + \omega_n^2 + \Delta_n^2} \), where \( \Delta \) is the supercon-
ductor’s pairing energy and \( \gamma \) is McMillan’s parameter
controlling the strength of the proximity effect in the
normal layer and, hence, the Andreev reflection amplitude
\( a_{\alpha}(\omega_n) = i \Delta_n/(\omega_n + \sqrt{\omega_n^2 + \Delta_n^2}). \) For a weak proximity
effect with \( \gamma \leq \pi k_B T \ll \Delta \), the amplitude \( a_{\alpha}^2 \) is small \[42 \] and equation (8) assumes the form

\[
I_c = \frac{8e k_B T}{h} \sum_{n \geq 0} \frac{\Delta^2 \omega_n^2}{\omega_n^2 + \Delta^2} \Re \left( \frac{(h + i \omega_n)^2}{|h + i(\omega_n + \Gamma)|^2} \right),
\]

where the exponential factor results from the dynamical
phase \( 2E_L/h \omega_F \) accumulated in the Andreev circle,
introducing the Thouless energy \( E_L = h \omega_F/2L \).

Figure 4 shows the temperature dependence of \( I_c \) for
the spin-degenerate case \( (h = 0) \). In the absence of tun-
neling \( (\Gamma = 0) \) it is just a monotonically exponential
decrease. However, for \( \Gamma \neq 0 \) the interplay of the trans-
mition antiresonance and the exponential suppression

FIG. 3: Critical current vs. temperature for a spin-
degenerate edge state: \( h = 0, \gamma = 0.1 E_L, \Delta = 10 E_L \). The
current is normalized to the value \( I_c(T_{\text{min}}) \) where \( T_{\text{min}} = 0.05 E_L/k_B \) is the lowest temperature for which the condition
\( \gamma \leq \pi k_B T \ll \Delta \) of weak proximity effect still holds.
FIG. 5: Critical current vs. temperature for a spin-polarized edge state: $h = 0.5E_L$, $\gamma = 0.1E_L$, $\Delta = 10E_L$.

gives rise to a maximum at finite $T$. Spin splitting of the graphene edge state lifts the Fano resonance condition $E = 0$ for both electron and Andreev reflected hole. Therefore, for relatively weak tunneling coupling, when $\pi k_B T \leq \Gamma < E_L$, the critical current increases with $h$ [Fig. 4], a behavior quite unusual for Josephson junctions. Surprisingly, for stronger tunneling coupling ($\Gamma > E_L$) the function $I_c(h)$ becomes nonmonotonic with a rather broad region $h_1 \leq |h| \leq h_2 \approx \Gamma$ where $I_c$ is negative. The lower boundary $h_3 \approx \pi k_B T$ is set by the temperature and is much smaller than all $E_L$, $\Gamma$ and $\Delta$. The supercurrent reversal is a consequence of the spin-dependent phases acquired by both electron and hole due to scattering off the spin-polarized graphene edge, with negative values of $I_c$ implying a built-in $\pi$-phase difference in the ground state of a Josephson junction as opposed to 0-phase difference for $I_c > 0$. The $0-\pi$ transition can be driven by temperature as shown in Fig. 5. Such a $\pi$ state is known to occur in ferromagnetic junctions where the condensate function oscillates in space (see, also recent reviews 29, 30). The author is not aware of any earlier work predicting $0-\pi$ transitions due to spin-dependent Fano scattering. The main condition for this mechanism to work, i.e. $|h| > \pi k_B T$, can be met in the millikelvin region at modest external magnetic fields.

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