Common-path interference and oscillatory Zener tunneling in bilayer graphene p-n junctions

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Detailed Terms
Interference and tunneling are two signature quantum effects that are often perceived as the yin and yang of quantum mechanics: a particle simultaneously propagating along several distinct classical paths versus a particle penetrating through a classically inaccessible region via a single least-action path. Here we demonstrate that the Dirac quasiparticles in graphene provide a dramatic departure from this paradigm. We show that Zener tunneling in gapped bilayer graphene, which governs transport through p-n heterojunctions, exhibits common-path interference that takes place under the tunnel barrier. Due to a symmetry peculiar to the gapped bilayer graphene bandstructure, interfering tunneling paths form conjugate pairs, giving rise to high-contrast oscillations in transmission as a function of the gate-tunable bandgap and other control parameters of the junction. The common-path interference is solely due to forward-propagating waves; in contrast to Fabry–Pérot-type interference in resonant-tunneling structures, it does not rely on multiple backscattering. The oscillations manifest themselves in the junction I–V characteristic as N-shaped branches with negative differential conductivity. The negative dI/dV, which arises solely due to under-barrier interference, can enable new high-speed active-circuit devices with architectures that are not available in electronic semiconductor devices.

Quantum tunneling through two or more barriers that are placed closely together is characterized by transmission that is sharply peaked about certain energies. Such “resonant-tunneling” effect arises because particles can reflect between the barriers and resonate at particular energies, allowing enhanced transmission through the barriers. This resonance phenomenon is similar to that taking place in optical Fabry–Pérot resonators. Resonant tunneling is particularly desirable in applications because it can give rise to negative differential resistance—current that goes down as voltage goes up—an interesting behavior that can be harnessed to form new devices (1, 2).

Here we propose an entirely different approach to realize oscillatory transmission, which involves only forward-propagating waves and a single barrier, and thus is distinct from the Fabry–Pérot interference of waves undergoing multiple reflection between two barriers. This behavior arises in graphene bilayer (3, 4), a two-dimensional semiconductor material with unique electronic properties, such as the field effect and the possibility of a particle simultaneously propagating along several distinct classical paths versus a particle penetrating through a classically inaccessible region via a single least-action path. Here we demonstrate that the Dirac quasiparticles in graphene provide a dramatic departure from this paradigm. We show that Zener tunneling in gapped bilayer graphene, which governs transport through p-n heterojunctions, exhibits common-path interference that takes place under the tunnel barrier. This behavior arises in the theory of p-n junctions in gated gapless graphene sheets (21), with a momentum component along the p-n interface playing the role of a bandgap.

The origin of the oscillatory behavior can be elucidated by a semiclassical analysis of the dynamics in the barrier region. In contrast to the standard case of tunneling through a one-dimensional barrier, where a unique saddle-point trajectory in a classically forbidden region is found for each energy, here we obtain multiple trajectories. Further, the trajectories form pairs with complex conjugate Wentzel–Kramers–Brillouin (WKB) action values S and S*. Common-path interference of such pairs gives rise to an oscillatory transmission

$$T = \left| a e^{-iS} + a^* e^{-iS^*} \right|^2 = 4|a|^2 e^{-iS} \cos^2 \left( \frac{S'}{\hbar} + \varphi \right),$$

where $$S = S' + iS''$$. Both $$S'$$ and $$S''$$ are monotonic functions of the bandgap and field strength (see Eq. 4). The oscillations in transmission will manifest themselves through negative differential conductivity in the I–V characteristic.

This unique behavior opens a door for designing new device architectures. Small intrinsic capacitance of planar heterojunctions can enable high-speed devices. Further, the single-particle effects responsible for the negative dI/dV are completely insensitive to the behavior in the doped regions, which is a distinct advantage compared to many resonant-tunneling devices (1) whose performance is limited by their relatively high capacitance and by thermal stability of dopants.
Model: The WKB Analysis
To clarify the origin of Eq. 1, we first consider transmission using the WKB formalism. Gapped BLG in the presence of a barrier potential \( V(x) \) is described by a \( 2 \times 2 \) quadratic Dirac Hamiltonian (4),
\[
H = \left( \frac{\Delta}{2m} (p_x - ip_y)^2 - \Delta \right) + V(x), \quad \Delta = \frac{E_g}{2} \tag{2}
\]
where \( E_g \) is the bandgap. We seek the wavefunction in the barrier region in the form
\[
\psi(x) \propto e^{i \int_{x_0}^{x} p(y) \, dy} \chi
\]
where \( \chi \) is a two-component spinor. The \( x \) dependence of momentum can be found from the energy integral \( E = \pm \left[ p_x^2 / 2m \right] + \Delta^{1/2} + V(x) \). In the barrier region, \( -\Delta < V(x) - E < \Delta \), this relation gives four complex roots
\[
p_s(x) = \pm \sqrt{-p_x^2 \pm 2mi \sqrt{\Delta^2 - (V(x) - E)^2}}, \tag{3}
\]
where \( p_s \) is a conserved \( y \) component of momentum. Two of the roots (3) have \( \text{Im} > 0 \), and the other two have \( \text{Im} < 0 \). Positive (negative) \( \text{Im} \) correspond to decaying (growing) exponentials which describe particle propagation to the right and to the left, respectively.

Focusing on the uniform-field model \( V(x) = -Fx \) (see Fig. 1, Inset) and for simplicity setting \( p_s = 0 \), we select from (3) the right-propagating solutions: \( p_s(x) = (i \pm 1) m^{1/2} \Delta^{1/2} - Fx + E_{\pm} / F^{1/4} \). These two solutions give complex conjugate WKB transition amplitudes \( e^{S1/2}, e^{-S1/2} \), where
\[
S, S' = (1 \pm i)an^{1/2} \Delta^{3/2} / F \tag{4}
\]
with the prefactor expressed through the Euler beta function, \( a = B(\frac{1}{4}, \frac{1}{2}) \approx 1.75 \).

The total transmission amplitude in the WKB approximation is the sum of the transmission amplitudes for the two decaying exponentials. Combining the contributions of the trajectories \( p_s(x) \), we can write the WKB wavefunction in the barrier region as a sum
\[
Ae^{i \int_{x_0}^{x} p_s(y) \, dy} + a^*e^{i \int_{x_0}^{x} p_s(y) \, dy}. \tag{5}
\]
Interference between these evanescent solutions produces an oscillatory transmission amplitude
\[
A = ae^{-S/2} + a^*e^{-S'/2}. \tag{5}
\]
Because \( \text{Re}S = \text{Re}S' \) and \( \text{Im} = -\text{Im}S' \), the two contributions to the transmission amplitude are of equal magnitude and differ in phase by \( \Delta = 2(\frac{1}{4} \text{Im}S - \varphi) \). Here, \( \varphi = \arg(a) \) is a phase offset between the two decaying exponentials, which can in principle be obtained by matching solutions at the classical turning points, but in practice is more easily obtained through a numerical procedure, which gives \( \varphi \approx \pi / 2 \) (see Fig. 2 and accompanying discussion).

For certain nodal values of \( F \) and \( \Delta \), the interference is destructive and the transmission probability vanishes. Plugging the values (4) in Eq. 5, we see that the transmission probability \( T = |A|^2 \) oscillates, going through nodes when \( an^{1/2} \Delta^{3/2} / Fh \) is an integer multiple of \( \pi \). This condition gives the nodal values
\[
\Delta_n = (an / a)^{1/3} (F^2 A^2 / m)^{1/3}, \quad n = 1, 2, 3, \ldots \tag{6}
\]
that match closely the nodes found numerically (Fig. 1). The dip in transmission at \( E_g = 0 \) originates from the chirality-assisted suppression of tunneling in gapless BLG (see ref. 22).

The oscillations in transmission, being a general feature deriving from interference, are a robust and generic phenomenon. In particular, the oscillations do not require a linear potential in the barrier region, and the WKB analysis may be straightforwardly generalized to an arbitrary potential profile \( V(x) \). Weak perturbations to the BLG dispersion also can be easily incorporated in the above analysis and shown not to matter as long as the perturbation strength is weak compared to the gap \( \Delta \). For example, the trigonal warping interaction can affect the dispersion within a few millielectronvolts of the Dirac point (4), thus its effect will be small in systems with gate-induced gap that can reach a few hundred millielectronvolts (7).

Fig. 1. Zener tunneling and common-path interference in BLG in the uniform-field model. Interference of two least-action tunneling paths results in oscillations, \( n = 1, 2, \ldots \). Shown is transmission at normal incidence, \( p_s = 0 \), as a function of bandgap size, in units \( \Delta_n = (Fh^2 / 2m)^{1/3} \) (semilog scale). Numerical results (red symbols), obtained by integrating Eq. 8, agree with the WKB result, Eqs. 1 and 4 (blue curve) in the entire range of \( \Delta \), large and small. Inset shows schematic setup of p-n junction: The bandgap \( E_g = 2\Delta \), the linear barrier potential \( V(x) = -Fx \) (see Eq. 2), and a pair of interfering tunneling paths.

Fig. 2. Evolution of a two-level system slowly driven through an avoided level crossing, Eq. 8. Nonadiabatic transitions between different levels, corresponding to Zener tunneling, take place in the Larmor precession region \( -p_\Delta \leq p \leq p_\Delta \), where \( p_\Delta = \sqrt{2m\Delta} \). Shown are adiabatic energy levels of the Hamiltonian, Eq. 8 (blue line) and schematic partition into regions of adiabatic evolution and Larmor precession.
Another requirement on experimental systems in which the interference phenomena described above can be realized is that of ballistic transport in the p-n junction region. Recent observation of Fabry–Pérot (FP) oscillations in graphene p-n-p junctions (24) provides a clear signature of ballistic transport in this system. The oscillation could be seen for the p-n interface separation of up to 60 nm, which sets a lower bound on the mean free path in the presence of a top gate. For a rough estimate, writing $F = U/L$ with $U$ a gate-induced potential difference across a p-n junction and $L$ the junction width (see Fig. 3, Inset), from Eq. 6 we predict the number of experimentally accessible nodes

$$n \approx \frac{am^{1/2} \Delta^{1/2}}{\pi \hbar} = \frac{\alpha \Delta L}{\pi \sqrt{2 eU \Delta}}, \quad \Delta = \frac{\hbar}{\sqrt{2m\Delta}}. \quad [7]$$

For $\Delta = 100$ meV, and using the effective mass in BLG $m = 0.033 m_0$, we estimate the characteristic lengthscale $\ell_\Delta \approx 3.18$ nm. Taking $eU = 4\Delta$ and $L = 60$ nm, we arrive at $n \approx 4$, which indicates that oscillatory Zener tunneling is well within reach of current experiments.

**Discussion: Zener Tunneling in Momentum Space.**

We now explain the origin of the oscillations from a different perspective, by mapping the transmission across the p-n junction to evolution of a two-level system which is swept through an avoided level crossing. This alternative formalism is specialized for the uniform-field model, and thus is less general than the WKBE method. However, it provides intuition and affords an avoided level crossing. This alternative formalism is specialized to evolution of a two-level system which is swept through an avoided level crossing, as illustrated in Fig. 2. Interband transitions are described by the process in which a state that started off in the $\sigma_1 = -1$ eigenstate at $p_x = -\infty$ will evolve into the $\sigma_1 = +1$ eigenstate at $p_x = +\infty$. The evolution is near-adiabatic at small $F$, with Zener tunneling described as (nonadiabatic) transitions across the gap.

In this framework, the oscillations in transmission can be understood in a simple and intuitive way by noting that the Heisenberg evolution of momentum $p_x(t)$ corresponds to sweeping through the avoided crossing at a constant speed, $dp_x/dt = F$. Comparing different terms in Eq. 8, we conclude that transitions may only happen in the region $-p_x < p_x < p_x$, where $p_x = \sqrt{2m\Delta}$ (see Fig. 2), whereas outside this region the evolution is adiabatic (here we set $p_0 = 0$ for simplicity). In the transition region, the dominant term in the Hamiltonian is $\Delta \sigma_3$. Spin rotation caused by this term can be described as Larmor precession about the $z$ axis by an angle $\delta \theta = (\Delta / \hbar^2)p_x, \Delta$. Periodic modulation of the transition rate of the form $\cos \delta \theta$, resulting from Larmor precession, leads to an estimate of the oscillation period that agrees with the WKB result, Eqs. 1 and 4.

The momentum-sweep analysis also helps to understand the dramatic difference in transmission between bilayer junctions and single-layer junctions. The latter problem can be mapped (26) to a canonical Landau Zener problem of a linear sweep through an avoided level crossing, for which transmission is a monotonic function of control parameters exhibiting no oscillations. This result is in agreement with the theory of p-n junctions in single-layer graphene (21).

In light of this analogy, it is interesting to compare our Larmor-type oscillations with the St"uckelberg oscillations arising in systems that are swept multiple times through a level crossing (27). Because our oscillations occur in a single sweep, they are more robust to dephasing and decoherence. Whereas St"uckelberg oscillations occur when the system remains phase coherent between consecutive sweeps, here only phase coherence over the timescale of a single sweep is necessary.

**Results: The $I$–$V$ Characteristic.**

We now place this discussion on a firm quantitative ground by calculating the transition probability numerically. We solve the differential equation, Eq. 8, in a suitably chosen interval $p_{\min} < p_x < p_{\max}$ taking as the initial state at $p_x = p_{\max}$ the adiabatic ground state. From the numerical solution, we determine the probability to evolve into the excited state at $p_x = p_{\min}$. The transmission probability, obtained in this manner for $p_{\max} = 0$ and $p_{\max} = \pm 22p_\Delta$, is shown in Fig. 1. The results are compared with the prediction of the WKB approach, Eq. 1, treating the pre-factor $|\psi|^2$ and the phase $\phi$ as fitting parameters. As illustrated in Fig. 1, excellent agreement is found for the values $\phi = 1.6$ and $|\psi|^2 = 0.78$ (which are tantalizingly close to $\pi / 2$ and $\pi / 4$), indicating that the WKB analysis provides reliable results.

Integrating Eq. 8 at finite $p_x$, we find that the transmission oscillates and vanishes at nodal values of $\Delta$ in pretty much the same way as for zero $p_x$. Comparing to the WKB analysis, which continues to apply at finite $p_x$, we find that the WKB phase offset $\phi(p_x)$ varies only weakly with $p_x$. Using this numerical procedure, we may also straightforwardly take into account trigonal warping.

Apart from a weak washing out of the nodes, we find no significant effect on the oscillations of transmission provided the trigonal warping energy scale is less than the gap size.

Next, we proceed to show that the oscillatory tunneling reveals itself through distinct features in the $I$–$V$ characteristic. The net tunneling current can be expressed, according to the Landauer
formula (14), as a sum of contributions of all conducting channels multiplied by energy distribution in reservoirs, giving

\[ I = \frac{e}{h} \int_{-\infty}^{\infty} dE (n_{E^{-}} - n_{E^{+}}) T(F). \]  

(9)

\[ T(F) = \frac{NW}{2\pi h} \int_{-\infty}^{\infty} dp \rho_p T_{p,E}(F). \]  

(10)

where \( W \) is the total length of the p-n interface, and the factor \( N = 4 \) is spin/valley degeneracy in BLG. Here, accounting for the fact that transmission is dominated by small values of \( p_y \) (see below), we treat the occupation numbers as \( p_y \) independent and factor out the quantity \( T(F) \), the net transmission integrated over \( p_y \).

Continuing to work with the uniform-field model, we treat transmission as energy independent and incorporate the source-drain voltage in the effective barrier potential via \( F = F_0 + eV_{ad}/L \) (see Fig. 3, Inset). Integrating over energies, we have

\[ I = \frac{e^2}{h} V_{ad} T(F_0 + eV_{ad}/L), \quad F_0 = eU/L. \]  

(11)

The dependence of transmission \( T_p \) on \( p_y \) may be found from Eq. 1 with \( S(p_y) \) and \( S'(p_y) \) evaluated using Eq. 3. Because the transmission is exponentially small in the barrier width, and the width of the barrier region grows monotonically with \( p_y^2 \), the net transmission \( T \) is dominated by small values of \( p_y \). Hence, we may approximate \( S \) and \( S' \) as

\[ SS' = \int_{-\infty}^{\infty} \frac{2|\alpha|^2 F^1/2}{(\alpha a^2 \Delta)^{1/2}} e^{-\tilde{\alpha} F} \left[ 2^{1/2} + \cos \left( \frac{2}{h} S'' + \tilde{\phi} \right) \right]. \]  

(12)

where \( \tilde{\phi} = 2\varphi - \frac{\pi}{4} \) and \( S'' \) are given by Eq. 4. Based on numerical results, we ignored the \( p_y \) dependence of the phase offset \( \varphi \) in Eq. 1. Interestingly, the resulting \( I-V \) curve, Eq. 11, exhibits negative differential conductivity.

A more accurate result for the net transmission \( T \) can be obtained by numerical integration of the exact WKB transmission over momenta (SI Appendix). In that, the full dependence of \( S \) and \( S' \) on \( p_y \) is retained, and also the contribution of the classically forbidden regions \( \Delta < |Fx - E| < \sqrt{\Delta^2 + (p_y^2/2m)^2} \) is included, which is of subleading order in \( p_y^2 \).

The resulting \( I-V \) dependence is shown in Fig. 3 for several values of the “built-in” (gate-induced) potential difference across the p-n junction. Notably, the \( I-V \) characteristic combines features of the Zener diode (sharp rise of current above current breakdown voltage) with N-shaped branches on which the differential conductivity is negative, resembling the resonant-tunneling (Esaki) \( I-V \) characteristic (23). Unlike the Esaki characteristic, the N-shaped branches occur simultaneously on the forward and reverse parts of the \( I-V \) dependence. The N-shaped features arise from oscillations in single-particle transmission, a mechanism very different from that leading to negative \( dl/dV \) in the Esaki diode. The valleys of current in Fig. 3 correspond to nodes of transmission (\( n = 1 \) in Fig. 1).

Conclusions

The p-n junctions of the type considered here can be realized using a configuration of gates which is already employed in current experiments (6, 24, 28, 29). A minimal configuration is a dual-gate geometry with a wide back gate and a narrow top gate, such as that used in the work on FP oscillations (24). Charging the two gates with voltages of opposite polarity, a bandgap can be induced under the top gate and, simultaneously, carrier density can be adjusted in the outer region. Applying source-drain bias will produce \( V_{ad} \)-dominated lateral electric field across the gapped region, corresponding to the regime \( U \ll V_0 \) where the effect of oscillations is most prominent (see Fig. 3). In addition, a built-in field \( U \) can be induced by selective doping or by a third gate.

In summary, transport in BLG p-n junctions is governed by common-path interference under the tunnel barrier. Unlike Fáy-Pérot interference that stems from multiple reflection between barriers, our interference effect involves only forward-propagating paths and a single barrier. The interference produces nodes in transmission as a function of the gate-tunable bandgap and other control parameters, leading to an \( I-V \) characteristic that features N-shaped branches with negative differential conductivity. Low capacitance of lateral heterojunctions can enable high-speed operation. The single-particle origin of negative \( dl/dV \) makes it insensitive to the behavior in the doped regions, unlike many resonant-tunneling devices where performance is limited by thermal stability of the dopants (1). We envision that BLG p-n junctions, owing to their multiple functionality and design simplicity, will become an integral part of the future graphene electronics toolkit.