Electronic cloaking of confined states in phosphorene junctions

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Abstract
We study the electronic transport of armchair (AC) and zigzag (ZZ) gated phosphorene junctions. We find confined states for both direction-dependent phosphorene junctions. In the case of AC junctions confined states are reflected in the transmission properties as Fabry–Pérot resonances at normal and oblique incidence. In the case of ZZ junctions confined states are invisible at normal incidence, resulting in a null transmission. At oblique incidence Fabry–Pérot resonances are presented in the transmission as in the case of AC junctions. This invisibility or electronic cloaking is related to the highly direction-dependent pseudospin texture of the charge carriers in phosphorene. Electronic cloaking is also manifested as a series of singular peaks in the conductance and as inverted peaks in the Seebeck coefficient. The characteristics of electronic cloaking are also susceptible to the modulation of the phosphorene bandgap and an external magnetic field. So, electronic cloaking in phosphorene junctions in principle could be tested through transport, thermoelectric or magnetotransport measurements.

Keywords: electronic cloaking, confined states, phosphorene junctions

Supplementary material for this article is available online (Some figures may appear in colour only in the online journal)

1. Introduction
Cloaking effect consists in making objects invisible to radiation, acoustic waves, matter waves, heat and charge fluxes, among others [1–5]. The typical cloaking effect is based on guiding plane waves around an object. The effect also refers to hiding an object in space. Cloaking effect is a phenomenon that can have a plethora of applications such as mantle cloaking, antennas, invisible sensors that do not perturb the field that they measure, etc [1]. With the arrival of 2D materials, in particular graphene, there were reports of the cloaking effect in bilayer graphene junctions [6–8] and graphene nanoribbons [9]. Experimental evidence based on transport measurements was also reported about this exotic phenomenon [10].

The so-called electronic cloaking is owing to the chirality mismatch of states outside and inside a bilayer graphene junction. In fact, electrons impinging onto the potential barrier at normal incidence can tunnel through it as if no localized states were available in their way. Until now there is no evidence of electronic cloaking effect in other 2D materials.

Phosphorene is a 2D semiconductor composed of two atomic layers arranged in a puckered honeycomb lattice. Its experimental fabrication was realized in 2014 by the mechanical exfoliation technique [11–13]. The phosphorene band structure is anisotropic, with the armchair (AC) and zigzag (ZZ) as fundamental directions, and a direct bandgap at the Γ point [14, 15]. By nanostructuring phosphorene with top gate electrodes, it is possible to obtain the so-called gated phosphorene junctions (GPs) [16, 17]. In fact, several phenomena have been reported in GPs [18–26]. For instance, negative
reflection and super-anti Klein tunneling [18], the spin Hartman effect [19], a direct-indirect-direct bandgap transition via elastic strain [20], a topological phase transition mediated by a transverse electric field in phosphorene nanoribbons [21, 22], among others. These characteristics rise the prospects of phosphorene from both the fundamental and technological standpoint [12, 15, 26, 27].

In this work, we show that electronic cloaking is also possible in phosphorene. To this end, we study the electronic transport of GPJs along the AC and ZZ direction. We find electronic cloaking in the ZZ direction, while in the AC direction the confined states manifest as Fabry–Pérot resonances in the transmission. We also analyze the hallmarks of the electronic cloaking on the transport properties, including the effects of the bandgap modulation and an applied magnetic field.

The rest of the paper is organized as follows: in section 2 the details of the low-energy effective Hamiltonian, the fundamentals of the hybrid matrix method as well as the transport formalism are given; in section 3 we show and discuss the most relevant results of the transmission and transport properties in GPJs, paying attention to the electronic cloaking along the ZZ direction; we end with our concluding remarks in section 4.

2. Method and formalism

GPJs can be fabricated by placing electrostatic gates over the phosphorene layer as shown in figures 1(a) and (c) [16, 17]. In the case of AC-GPJs, the charge carriers propagate along the x-direction and the electrostatic gate is oriented in the transverse direction, vice versa for ZZ-GPJs. The electrostatic gate induces a potential barrier by shifting the electronic structure, figures 1(b) and (d).

The electronic transport in GPJs can be modeled with the tight-binding low-energy effective Hamiltonian [14, 18, 28–30]

\[ H = \begin{pmatrix} V(x) & g^*(k) \\ g(k) & V(x) \end{pmatrix}, \]

where \( g(k) = \Delta + \frac{\hbar^2}{2m_x} + i\nu p_x \), \( m_x = 2\hbar^2 / (t_1 a^2 + 2\delta(2t_1 a - \Delta)) \), \( \delta = -2\hbar^2 / (t_1 b^2) \), \( \nu = (t_1 a - \Delta) / \hbar \), \( t_1 = -1.22 \) eV and \( t_2 = 3.665 \) eV are the hopping energies between the first and second nearest neighbors [30], \( 2\Delta = 4t_1 + t_2 = 2.45 \) eV is the direct band gap, \( a = 4.42 \) Å and \( b = 3.27 \) Å are the distance of the orthogonal phosphorene basis, \( \delta = 0.8 \) Å is the distance between the two atoms in the unit cell, and \( V(x) \) is the potential barrier that can correspond to AC-GPJs, \( V(x) = V_0 \) or ZZ-GPJs, \( V(x) = V_0 \), \( V_0 \) being the strength of the electrostatic potential. The dispersion relation in the potential barrier region is given by

\[ E = V_0 \pm \sqrt{\left( \Delta + \frac{\hbar^2 q_x^2}{2m_x} + \frac{\hbar^2 q_y^2}{2m_y} \right)^2 + v^2 \hbar^2 q_z^2}. \]

The transmission is obtained with the help of the numerical stable band matrix method [31]. This method consists in rewrite the eigenvalue problem \( H\psi = E\psi \) as Sturm–Liouville matrix equation [32].

\[ L(x) \cdot \mathbf{F}(x) \equiv dA(x)/dx + Y \cdot d\mathbf{F}(x)/dx + W(x) \cdot \mathbf{F}(x), \]

where \( \mathbf{F}(x) \) is the wave function or field, \( \mathbf{A}(x) = \mathbf{B}(x) \cdot d\mathbf{F}(x)/dx + \mathbf{P}(x) \cdot \mathbf{F}(x) \) is the linear differential form, and \( Y(x), W(x), \mathbf{B}(x), \mathbf{P}(x) \) are coefficient matrices [32]. This equation and the mathematical process that we will outlined correspond to AC-GPJs. However, a similar equation and process apply for ZZ-GPJs. As we are dealing with a constant potential the solution to the Sturm–Liouville matrix equation can be obtained straightforwardly. The general solution is given by

\[ \mathbf{F}(x) = \sum_{i=0}^{4} a_i \mathbf{F}_i(x), \]

\[ \mathbf{A}(x) = \sum_{i=0}^{4} a_i \mathbf{A}_i(x), \]

where \( \mathbf{F}(x) = \mathbf{F}_0 e^{i\xi_1 x} \) and \( \mathbf{A}_i(x) = \mathbf{A}_0 e^{i\xi_i x} \) with amplitudes \( \mathbf{F}_0 = (\phi_0, \varphi_0)^T = (\phi_0^*(k), E - V_0)^T \) and \( \mathbf{A}_0 = (\alpha_0, \beta_0)^T = (-i\hbar/2 + i\eta a^2/2m_\nu)(E - V_0), (i\hbar/2 - i\eta a^2/2m_\nu)\beta_0 \). The eigenvalues \( q_i \) \( (i = 1, 2, 3, 4) \) are given by

\[ q_1 = \sqrt{-\xi_1 + \xi_2}, \quad q_2 = -q_1, \quad q_3 = i\sqrt{-\xi_1 + \xi_2}, \quad q_4 = -q_3, \]

with \( \xi_1 = 2m_\nu a^2/\hbar^2 + (2m_\nu/a^2)(\Delta + \hbar^2 q_z^2/2m_\nu) \). \( \xi_2 = (2m_\nu/a^2) \sqrt{(E - V_0)^2 + m_\nu^2 a^4/4 + 2m_\nu a^2(\Delta + \hbar^2 q_z^2/2m_\nu)} \). As we can notice, there are two propagating waves and two evanescent-divergent waves. The solutions in the left and right semi-infinite regions can be obtained readily by taking \( V_0 = 0, q_i \to k_i, \) and \( q_j \to k_j \).
different regions of our system we can define the hybrid matrix as [31, 32]:

\[
\begin{bmatrix}
F_L(x_i) \\
A_R(x_i)
\end{bmatrix} = H(x_i, x_r) \cdot \begin{bmatrix}
A_L(x_i) \\
F_R(x_i)
\end{bmatrix},
\]

(6)

where \( H(x_i, x_r) \) is the hybrid matrix of the phosphorene junction evaluated at the boundaries of the electrostatic barrier. The field and linear differential form of the left–right semi-infinite region \( F_{L,R}(x_i) \) and \( A_{L,R}(x_i) \) are also evaluated at the boundaries \( x_{L,R} \). Equation (6) can be written in terms of the transmission and reflection amplitudes as follows

\[
\begin{bmatrix}
L_2/L_1 \\
L_4/L_1 \\
R_1/L_1 \\
R_3/L_1
\end{bmatrix} = [M_1 - H(x_i, x_r) \cdot M_2]^{-1}[H(x_i, x_r) \cdot M_3 - M_4],
\]

(7)

where \( M_1, M_2, M_3, \) and \( M_4 \) are auxiliary matrices [31, 32]. Finally, the transmittance can be calculated as

\[
T = |R_1/L_1|^2,
\]

(8)

The conductance is evaluated using the relation

\[
G(E) = G_0 \int_{q_{\min}}^{q_{\max}} T(E, q) dq,
\]

(9)

where \( q \) is the transverse wave vector component, \( G_0 = \hbar^2/\pi e^2 \) is the fundamental conductance factor, with \( L \) the width of the system in the transverse direction. The integral runs over the interval \( q_{\min} < q < q_{\max} \). In the case of AC-GPJs \( q = k_x \) and \( L = L_x \), while for ZZ-GPJs \( q = k_x \) and \( L = L_y \).

3. Results and discussion

As we can notice in figures 1(c) and (d) by considering an appropriate electrostatic potential we can bring hole states inside the barrier of AC- and ZZ-GPJs. In principle, these states will participate in the electronic transport with direct hallmarks in the transmission and conductance. In fact, in the case of AC-GPJs there are transmission resonances at normal \((k_x = 0)\) and oblique \((k_x \neq 0)\) incidence, see figures 2(a) and (c). The transmissions maps also corroborate plenty of these resonances in the energy range \(1.3 \text{ eV} < E < 2.8 \text{ eV}\) arranged in semi-circular fashion, see figures 3(a) and (c). The number of resonances at normal incidence coincides with the number of semi-circular regions in the transmission maps. If we fixed \( V_0 \) and change \( d_B \) the number of resonances/semi-circular transmission regions changes as well. For instance, in the case of \( V_0 = 4 \text{ eV} \) and \( d_B = 1, 3 \) and \( 5 \) nm the number of resonances/semi-circular regions is \( 1, 3 \) and \( 5 \) respectively, see figure S1 (https://stacks.iop.org/JPCM/34/195301/mmedia) in the supplementary information. The conductance also manifests hallmarks associated to the hole states inside the barrier. In particular, the conductance presents sharp peaks located close to the energies of the transmission resonances at normal incidence and that in number correspond to the number of resonances/semi-circular transmission regions, see figures 4(a), (c) and (e). Another quantity that also shows hallmarks of the hole states inside the barrier could be helpful experimentally is the Seebeck coefficient \( S = \frac{\pi k_B T}{n e} \frac{\partial \ln G(E)}{\partial E} |_{E_{\text{F}}}, \) where \( k_B \) is the Boltzmann constant, and \( T \) is the average temperature in the thermoelectric device [33]. As we can see in figures 4(b), (d) and (f), the Seebeck coefficient shows oscillations in the energy range \(1 \text{ eV} < E < 3 \text{ eV}\), which correspond with the resonances presented in the transmission at normal incidence and with the sharp peaks in the conductance. Similar results are obtained if \( d_B \) is fixed and \( V_0 \) is varied, see figure S2 in the supplementary information.

In the case of the ZZ direction, the electronic transport has been overestimated due to the charge carriers in this direction have been regarded as Schrödinger particles [18, 29]. However, Jung et al [34] have demonstrated that in reality the charge carriers in phosphorene possess a special pseudospin texture. The pseudospin is a characteristic of two-level quantum systems such as honeycomb lattices [35]. The pseudospin is involved in most of the exotic properties of 2D materials, including the electronic cloaking in bilayer graphene [6, 10].

The electronic cloaking can be understood with the help of the eigenbasis of \( \sigma \), denoted by \( \varphi_+ \) and \( \varphi_- \). In this basis the eigenvalue equation \( H \psi = E \psi \) results in a system of coupled equations. The coupling between \( \varphi_+ \) and \( \varphi_- \) is suppressed at normal incidence \((k_x = 0)\),

\[
\frac{d^2}{dy^2} - \frac{2m_e}{\hbar^2} (\Xi E \pm V_0 + \Delta) \varphi_\pm(y) = 0.
\]

(10)

\( \varphi_+ \) states represent states that transmit through the potential barrier \( V_0 \), while states \( \varphi_- \) represent confined states inside the potential well \(-V_0\). As a result of the decoupling between \( \varphi_+ \) and \( \varphi_- \) at normal incidence, \( \varphi_+ \) states tunnel through the barrier without interaction with the confined states \( \varphi_- \).
Figure 3. Transmission maps as a function of the energy and the transverse wave vector for (a) AC- and (b) ZZ-GPJs. (c) and (d) Correspond to zooms of (a) and (b), respectively. The structural parameters of the gated junctions are the same as in figure 2.

Figure 4. Conductance (first column) and Seebeck coefficient (second column) as a function of the Fermi energy for AC-GPJs for different barrier widths as indicated. The strength of the electrostatic potential is $V_0 = 4$ eV.

Figure 5. Conductance (first column) and Seebeck coefficient (second column) as a function of the Fermi energy for ZZ-GPJs at different barrier width as indicated. The strength of the electrostatic potential is $V_0 = 4$ eV.

The barrier acts as a cloak for confined states blocking the transmission completely, i.e., electrons tunnel the barrier as if no localized states were available in their way. In the case of oblique incidence ($k_x \neq 0$), $\varphi_+$ and $\varphi_-$ are coupled, the resultant coupled equations conduce to a differential equation of fourth order. In this case, in the barrier region we have two propagating waves and two evanescent-divergent waves.

Our numerical calculations confirm the electronic cloaking of confined states in ZZ-GPJs. The transmission at normal incidence ($k_x = 0$) is totally suppressed in the energy region...
Figure 6. Transmittance (first row) and transmission maps (second row) as a function of the energy for AC- (first column) and ZZ-GPJs (second column) for the special case of zero bandgap ($\Delta = 0$). Conductance (third row) as a function of the energy for AC- (first column) and ZZ-GPJs (second column) for different band gaps $\Delta$ as indicated. The width of the barrier is $d_B = 3$ nm and the potential is $V_0 = 4$ eV.  

1.3 eV $< E < 2.8$ eV despite there are hole states inside the barrier, see figure 2(b). At oblique incidence ($k_x \neq 0$), the transmission presents six resonances in the mentioned energy region, see figure 2(d). We can also appreciate the electronic cloaking in the transmission maps. In figures 3(b) and (d) we can see transmission resonances arranged in semi-circular fashion as in the case of AC-GPJs, however the number of semi-circular regions is greater for ZZ-GPJs. The number of semi-circular regions correspond to the number of resonances in the transmission at oblique incidence. More importantly, the transmission is totally suppressed at normal and nearly normal incidence, manifesting the cloaking effect of the confined states. The transport properties also manifest hallmarks of the electronic cloaking. As we can see in the inset of figures 5(a), (c) and (e), the conductance shows several singular peaks (sharp L-shaped cusps), increasing in number as $d_B$ increases. Moreover, the energy position of the singular peaks coincides with the energy location of the invisible confined states, constituting a direct hallmark of electronic cloaking. These singular peaks are similar to the ones found in bilayer graphene as a hallmark of electronic cloaking [6]. However, in phosphorene it is not necessary to subtract any contribution to the conductance to observe the singular peaks. As we mentioned earlier an alternative quantity that can help to confirm the cloaking effect is the Seebeck coefficient. The electronic cloaking results in inverted (negative) spikes in the Seebeck coefficient as characteristic hallmark. We have identified them with red arrows in figures 5(b), (d) and (f). As we increase the barrier width the number of inverted spikes in the Seebeck coefficient increases as well, corresponding to the number of singular peaks in the conductance. Similar results are obtained if we fixed the barrier width and increase systematically the potential, see figure S3 in the supplementary information.

The modulation of the bandgap $2\Delta$ can give us information about the prevalence of the cloaking effect. In particular, it is instructive to know the modifications caused by closing the bandgap $\Delta = 0$. In the AC direction, the transmission is almost perfect at normal and near normal incidence when the bandgap is closed, similar to the perfect transmission (Klein tunneling) and collimation in graphene [36, 37], see figures 6(a) and (b). In the ZZ direction, the cloaking effect is preserved, that is, the transmission remains blocked at normal incidence, see figure 6(b). In addition, the number of semi-circular regions increases, as a consequence the number of invisible states increases as well, see figure 6(d). The conductance rises as the bandgap is reduced, and the sharp and singular peaks of...
Figure 7. Transmission maps of ZZ-GPJs as a function of the energy for different strengths of the applied magnetic field as indicated. The width of the barrier is \( d_B = 3 \text{ nm} \) and the potential is \( V_0 = 4 \text{ eV} \).

Figure 8. Conductance as a function of the energy for (a) AC- and (b) ZZ-GPJs when an external magnetic field is applied. The solid black, blue, red and violet curves correspond to magnetic fields of \( B = 0B_0, B = 5B_0, B = 10B_0 \) and \( B = 20B_0 \) respectively, with the reference field \( B_0 = 73.1 \text{ T} \). (c) and (d) Correspond to zooms of the low energy regions of (a) and (b). The width of the barrier is \( d_B = 3 \text{ nm} \) and the potential is \( V_0 = 4 \text{ eV} \).

AC- and ZZ-GPJs respectively smear as the bandgap closes, see figures 6(e) and (f).

We can also use an external magnetic field to see the prevalence of the cloaking effect and identifiable changes on the hallmarks of the electronic cloaking. An external magnetic field can be incorporated via the vector potential \( \mathbf{A} = \nabla \times \mathbf{A} \) by modifying the momentum vector \( \mathbf{p} \rightarrow \mathbf{p} + e\mathbf{A} \). We have considered a piecewise vector potential (deltaic magnetic field) acting on the same region as the electrostatic potential. For AC-GPJs the vector potential is \( A(x) = A_y \hat{y} = (0, B(B_0)l_B, 0) \), while for the ZZ-GPJs \( A(y) = A_x \hat{x} = (B(B_0)l_B, 0, 0) \). Here, \( l_B = \sqrt{\hbar/eB_0} \) is the magnetic length, and \( B_0 \) the strength of the reference magnetic field. In the case of ZZ-GPJs, the presence of the magnetic field suppresses the cloaking effect, shifting the semi-circular transmission regions until a transmission gap takes place at high magnetic fields, see figure 7. The applied magnetic field also transform the singular peaks of the conductance in sharp peaks, shifting them to higher energies and disappearing systematically with the magnetic field until a conductance gap is created at high magnetic fields, see figure 8. Similar results are obtained if in addition to the magnetic field the bandgap is closed, see figure S4 in the supplementary information. However, in this case we can choose wider barriers, smaller electrostatic potentials, and more importantly reasonable magnetic fields. In the case of AC-GPJs, the applied magnetic field is not as preponderant as for ZZ-GPJs, requiring stronger magnetic fields to see sizable changes in the transmission and transport properties, see figures 8 and 9.

Here, it is important to mention that the perfect reflection through the electrostatic barrier at normal incidence is one of the most prominent features of transport in phosphorene along
Figure 9. Transmission maps of AC-GPJs as a function of the energy for different strengths of the applied magnetic field as indicated. The width of the barrier is $d_0 = 3$ nm and the potential is $V_0 = 4$ eV.

the ZZ direction. The perfect reflection or anti-Klein tunneling is independent of the presence of the intrinsic bandgap or its manipulation. This result contrasts with graphene, where the anti-Klein tunneling is suppressed in the presence of a bandgap [38] or transformed in Klein tunneling by appropriately adjusting the bandgap [39, 40]. At oblique incidence the anti-Klein tunneling disappear due to the presence of Fabry–Pérot resonances. These resonances can be modulated by the electrostatic potential, the with of the barrier or with a magnetic field. Similar behavior can be found when a $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian is used [41]. The present results where obtained with the help of the tight-binding Hamiltonian given by equation (1), which is a well established Hamiltonian [14]. In this context, we hope that our findings motivate experimentalists to corroborate electronic cloaking in phosphorene and theoreticians to study the validity of the different phosphorene Hamiltonians.

Finally, we would like to remark some important points that could have a considerable impact on our findings. It is well-known that edge states play an important role in the quantum transport of phosphorene nanoribbons [21, 22]. In electrostatic barriers like ours edge states could be possible due to the mass contrast of the charge carriers outside and inside the barriers [42]. Moreover, an electrostatic barrier is a well for holes, and quantum wells have been instrumental for topological states [43, 44]. The relation between edge states and electronic cloaking is an interesting and open problem that requires a thorough and detailed analysis. Impurities and temperature effects could also play an important role in the electronic and transport properties of GPJs. If the band structure is affected, our description of the charge carriers (low-energy effective Hamiltonian) is no longer valid necessarily. In the case of the transport properties, impurities could reduce significantly quantities such as the mean free path. If it is the case, our transport regime (quantum coherent transport) is no longer valid, and the diffusive regime is needed to study the transport properties. Regarding temperature, we need to extend the formalism to compute the temperature-dependent conductance as well as the temperature-dependent Seebeck coefficient beyond the Cutler–Mott formula [33]. In general, it is expected that the singular and inverted peaks in the conductance and Seebeck coefficient be suppressed by temperature effects. Both impurities and temperature effects require a thorough assessment that goes beyond the aim and scope of the present study.

4. Conclusions

In conclusion, the highly directional-dependent pseudospin texture of the charge carriers in phosphorene results in electronic cloaking at normal incidence for ZZ-GPJs, while for AC-GPJs confined states manifest as Fabry–Pérot resonances in the transmission. The invisible confined states manifest themselves as singular peaks in the conductance and as inverted (negative) spikes in the Seebeck coefficient. The electronic cloaking is insensible to the modulation the bandgap and is suppressed with the application of a magnetic field. Furthermore, the peaks associated to the cloaking effect are smeared
with the bandgap modulation and the applied magnetic field. These characteristics can be used as a hallmark of the electronic cloaking in transport, thermoelectric or magnetotransport measurements.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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