Spatial Delocalization and Perfect Tunneling of Matter Waves: Electron Perfect Lens

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It is theoretically demonstrated that electron states in semiconductors or graphene can be perfectly transmitted through a complementary material with dual properties, independent of the angle of incidence. It is shown that such complementary material may also provide a strong spatial delocalization of bounded electronic states, changing dramatically the confinement of the wave function, and acting effectively as a lens for the probability wave. The results are the electron analogue of a perfect lens for electromagnetic waves proposed in an earlier work.

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The idea of perfect lensing [1,2] continues to fuel the imagination of the scientific community due to its groundbreaking and far-reaching implications in photonics, most notably the possibility of having imaging with a resolution not limited by the diffraction of light [3,4]. In particular, a slab of a material with double negative parameters $[\varepsilon(\omega_0) = \mu(\omega_0) = -1]$ standing in a vacuum may permit two remarkable things: (i) the perfect transmission and negative refraction of the photonic states of the vacuum (propagating modes at $\omega = \omega_0$), independent of the angle of incidence; (ii) the enhancement and the delocalization of the near field of a source, so that it is spread over a wide spatial region (beyond the perfect lens exit interface), rather than being confined to the immediate vicinity of source. The "perfect lens" idea has been mostly discussed in the context of electromagnetic waves, and its generalization to electronics received little attention, except for recent works on graphene [5,6]. Here, we unravel the general principles that enable the perfect tunneling and strong spatial delocalization of the stationary states of complementary materials described by the Hamiltonian formalism. We apply the developed theory to matter waves in graphene and semiconductor heterostructures.

As a starting point, we consider two bulk materials *A* and *B* that are modeled by a Hamiltonian of the form, $\hat{H}_i = \hat{H}_i(E, \mathbf{k})$ with $\mathbf{k} = -i\nabla$ with $\nabla_l = \partial_{x_l}$, and i = A, B. As detailed in Ref. [6], the Hamiltonian is allowed to be energy (*E*) dependent, because we want to adopt an effective-medium description of the pertinent wave phenomena (e.g., electron waves) based on an envelope function. The operators \hat{H}_i are independent of \mathbf{r} , since within an effective-medium approach the underlying granularity (e.g., the microscopic periodic electric potential of the ionic lattice) is hidden. We consider a global system such that [without loss of generality the interface is taken at x = 0, as shown in Fig. 1(a)]:

$$\hat{H} = \begin{cases} \hat{H}_A(E, -i\partial_x, -i\partial_y, \ldots), & x < 0\\ \hat{H}_B(E, -i\partial_x, -i\partial_y, \ldots), & x > 0 \end{cases}$$
(1)

Next, we show that in certain circumstances two Bloch stationary states of the sub-systems A and B may be paired to produce a stationary state, $(\hat{H} - E)\psi = 0$, of the global system. Since \hat{H} is defined in terms of branches to calculate the stationary states one needs to specify the boundary conditions at the interfaces. Here, we only consider materials such that at the energy level of interest the boundary conditions are *compatible* with

$$S_B \psi_B(0, y, z) = S_A \psi_A(0, y, z),$$
 (2a)

$$j_{x,B}(0, y, z) = j_{x,A}(0, y, z).$$
 (2b)

In the above, S_i represent some system-dependent multiplication (matrix) operators, and $j_{x,i}$ represents the *x* component of the probability current (i = A, B). For most cases S_i reduces to the identity operator, and in that case the boundary conditions reduce to the continuity of the envelope wave function at the interface and of the normal component of the probability current. We can enunciate the following result. *Lemma*: Suppose that for some fixed energy level *E*, and multiplication operators S'_A and S'_B , the Hamiltonians \hat{H}_A and \hat{H}_B satisfy

$$S'_{A}\hat{H}_{A}(E, k_{x}, k_{y}, \ldots)S^{-1}_{A} + S'_{B}\hat{H}_{B}(E, -k_{x}, k_{y}, \ldots)S^{-1}_{B}$$

= $E(S'_{B}S^{-1}_{B} + S'_{A}S^{-1}_{A}).$ (3)



FIG. 1 (color online). (a) The interface between two semiinfinite regions, such that the electron wave dynamics in each region is described by the operator \hat{H}_i , i = A, B. (b) Similar to (a) but for the case of two interfaces.

Then, any stationary state $\psi_A(\mathbf{r})$ of the subsystem *A* associated with the energy *E*, can be used to construct a stationary state ψ of the global system (\hat{H}), such that

$$\psi(\mathbf{r}) = \begin{cases} \psi_A(x, y, \ldots), & x < 0\\ \psi_B(x, y, \ldots), & x > 0 \end{cases}$$
(4)

with $S_B \psi_B(x, y, ...) \equiv S_A \psi_A(-x, y, ...)$, provided one of the following conditions is observed. *Case I*: The boundary condition 2(b) is automatically satisfied when 2 (a) is satisfied. *Case II*: The operators S_i and S'_i satisfy $S_B S'^{\dagger}_B = S_A S'^{\dagger}_A$ and the probability current is given by $j_x = \text{Re}\{\psi^*(1/\hbar)(\partial \hat{H}/\partial k_x)(E, \mathbf{k})|_{\mathbf{k}=-i\nabla}\psi\}.$

The proof of the Lemma is given in the Supplemental Material [7]. In what follows, we apply this theory to the scenario of Fig. 1(b), where the regions A and B have common boundaries at x = 0 and x = d. Let $\psi_A(\mathbf{r})$ be a stationary state of \hat{H}_A for the energy level E for which Eq. (3) is satisfied. Using the Lemma at the two interfaces, it is readily seen that the system represented in Fig. 1(b) has the stationary state

$$\psi(\mathbf{r}) = \begin{cases} \psi_A(x, y, \ldots), & x < 0\\ S_B^{-1} S_A \psi_A(-x, y, \ldots), & 0 < x < d . \\ \psi_A(x - 2d, y, \ldots), & x > d \end{cases}$$
(5)

At the second interface we applied the Lemma to the function $S_B^{-1}S_A\psi_A(-\tilde{x}-d, y, ...)$ with $\tilde{x} = x - d$, which is transformed into $S_A^{-1}S_BS_B^{-1}S_A\psi_A(+\tilde{x}-d, y, ...)$. In particular, if $\psi_A(x, y, ...) = \psi_0 e^{i\mathbf{k}\cdot\mathbf{r}}$ is a Bloch mode of the subsystem A, it is clear that this wave is transmitted with no reflections through the region 0 < x < d, and that the transmission coefficient T [defined so that $\psi_A(x = d, y, ...) = T\psi_A(x = 0, y, ...)$] is equal to $T = e^{-ik_x d}$. Thus, we have a "perfect tunneling" through the region B, independent of the angle of incidence.

As a first example, we consider the case of light waves. As discussed in Ref. [6], appendix B, the dynamics of the electromagnetic field in continuous media can be formulated in terms of a Schrödinger-type equation of the form $\hat{H}\psi = i\hbar(\partial/\partial t)\psi$ with $\psi = \mathbf{G}$ being a six-component vector written in terms of the electric displacement and magnetic induction fields, **D** and **B**, such that

$$\mathbf{G} = \begin{pmatrix} \mathbf{D} \\ \mathbf{B} \end{pmatrix}.$$

The operator \hat{H} is such that $\hat{H} = \hbar \hat{N} \cdot \mathbf{M}^{-1}$ with

$$\hat{N}(\mathbf{k}) = \begin{pmatrix} 0 & i\nabla \times \\ -i\nabla \times & 0 \end{pmatrix}$$

with $\mathbf{k} = -i\nabla$. The material operator **M** links the macroscopic fields as $\mathbf{G} = \mathbf{M} \cdot \mathbf{F}$ with

$$\mathbf{F} = \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix}.$$

In the frequency domain,

$$\mathbf{M}(\boldsymbol{\omega}) = \begin{pmatrix} \bar{\boldsymbol{\varepsilon}} & c^{-1} \bar{\boldsymbol{\zeta}} \\ c^{-1} \bar{\boldsymbol{\zeta}} & \bar{\boldsymbol{\mu}} \end{pmatrix}$$

reduces to a multiplication operator for the general case of a bianisotropic material. It should be mentioned that in this problem \hat{H} does not represent the energy of the system, and obviously ψ is not a probability density wave. The stationary states of the electromagnetic field are such $\hat{H}\mathbf{G} = \omega\mathbf{G}$, where for simplicity we put $\hbar = 1$. Based on the Lemma, we prove in the Supplemental Material [7] that at a fixed frequency ω_0 the general tunneling condition for two materials described by the material matrices \mathbf{M}_i (i = A, B) reduces to $\mathbf{M}_B(\omega_0) = -\tilde{\mathbf{R}}_x \cdot \mathbf{M}_A(\omega_0) \cdot \tilde{\mathbf{R}}_x$, where

$$\tilde{\mathbf{R}}_{x} = \begin{pmatrix} \mathbf{R}_{x} & 0\\ 0 & \mathbf{R}_{x} \end{pmatrix}$$

and $\mathbf{R}_x \mathbf{r} \equiv (-x, y, ...)$ is a reflection operator. For example, if the region *A* is taken as an isotropic material with $\varepsilon = \varepsilon_A$ and $\mu = \mu_A$ then the region *B* is required to have $\varepsilon_B = -\varepsilon_A$ and $\mu_B = -\mu_A$. We can immediately recognize as particular cases the results of Pendry [1] and Alù and Engheta [8]. Moreover, the case of anisotropic materials reduces to a result originally discovered in Ref. [2]. Our theory generalizes these results to the class of bianisotropic electromagnetic systems. Interestingly, in general the perfect tunneling condition may depend on the orientation of the interface.

As a second example, we consider a massless particle described by a generalized two-dimensional Dirac equation. Specifically, it is assumed that $(\hat{H}\psi)(E, \mathbf{k}) =$ $[\hbar v_F \boldsymbol{\sigma}_{ef} \cdot \mathbf{k} + V_{ef}(E)] \cdot \psi$, with $\mathbf{k} = -i(\partial_x, \partial_y)$ and $\boldsymbol{\sigma}_{ef} = \boldsymbol{v}_{xx} \boldsymbol{\sigma}_{x} \hat{\mathbf{x}} + \boldsymbol{v}_{yy} \boldsymbol{\sigma}_{y} \hat{\mathbf{y}}$, where \boldsymbol{v}_{ll} are constant parameters (independent of both E and k) and σ_l are the Pauli matrices (l = x, y). Moreover, it is supposed that the effective potential V_{eff} satisfies $V_{\text{eff}} = V_0 - \alpha (E - V_0)$ with $\alpha = v_{xx} - 1$ and V_0 is some constant. When $v_{ll} = 1$ this Hamiltonian may describe the dynamics of electrons associated with the K-Dirac cone in pristine graphene, v_F being the Fermi velocity [9,10]. We have recently shown that electron waves (associated with the K point of the Brillouin zone) in x-stratified graphene superlattices may be described by the general form of the Hamiltonian with $v_{ll} \neq 1$ [6]. In particular, when the anisotropy parameter $\chi = v_{yy}/v_{xx}$ is such that $|\chi| \ll 1$, the electron waves may be supercollimated along the x direction [6,11,12]. The perfect tunneling of electron waves in graphene superlattices predicted in Ref. [6] can be easily explained in the framework of the present theory. Indeed, let us assume that $\hat{H}_i = \hbar v_F \boldsymbol{\sigma}_{\text{eff},i} \cdot \mathbf{k} + V_{\text{eff},i}$ with i = A, B, and that the boundary conditions at the interfaces between the two materials are consistent with Eq. (2a) with S_A and S_B scalars. Taking $S'_i = \nu_{xx,i}^{-1} S_i$ it follows that Eq. (3) is satisfied provided $\hbar v_F(\chi_A + \chi_B) \sigma_y k_y + \nu_{xxA}^{-1} V_{ef,A} +$

 $\nu_{xx,B}^{-1}V_{ef,B} = E(\nu_{xx,A}^{-1} + \nu_{xx,B}^{-1}).$ Using the relation $\nu_{xx,i}^{-1} V_{\text{eff},i} = V_{0,i} + (\nu_{xx,i}^{-1} - 1)E$, we find that the tunneling condition is $\hbar v_F(\chi_A + \chi_B) \boldsymbol{\sigma}_{v} k_v = 2E - V_{0,A} - V_{0,B}$. This can only hold for an arbitrary wave vector if the energy level is $E = (V_{0,A} + V_{0,B})/2$, and if the anisotropy parameters of the two superlattices are symmetric $\chi_A = -\chi_B$, which is the result of Ref. [6]. Notice that we are in the conditions of the case I of the Lemma because for massless particles the boundary condition 2(a) is sufficient to match the pseudospinors at the two sides of the interface. It is also interesting to note that if the material A is pristine graphene then the material B is required to have $\chi_B = -1$. Thus \hat{H}_B is formally analogous to the Hamiltonian that describes the dynamics of electrons in pristine graphene close to the second Dirac cone (located at K'), within the Diracfermion approximation.

In the final example, we study the tunneling of matter waves in II-VI semiconductor heterostructures. The electronic structure of such heterostructures can be determined using the envelope-function approximation [13]. Within this approach, the effective Hamiltonian of a bulk semiconductor may be taken $\hat{H}(E, \mathbf{k}) = (\hbar^2/2)\mathbf{k} \cdot \mathbf{M}^{-1} \cdot \mathbf{k} +$ V, where V = V(E) and $\mathbf{M} = \mathbf{M}(E)$ are, respectively, the effective potential and the (energy dependent) effective mass [14]. Let us suppose that two lattice matched semiconductors—described by the parameters V_i and \mathbf{M}_i (i = A, B)—are paired. We assume that generalized Ben Daniel-Duke boundary conditions hold at the interfaces, so that the envelope function ψ and $\hat{\mathbf{x}} \cdot \mathbf{M}^{-1} \cdot \nabla \psi$ are continuous [13]. Thus, we take $S_i = S'_i = \hat{I}$ equal to identity operator in Eq. (2a), and hence, provided \hat{H}_i (i = A, B) satisfy $\hat{H}_A(E, \mathbf{k}) + \hat{H}_B(E, \mathbf{R}_x \mathbf{k}) = 2E$, we are in the conditions of case II of the Lemma. For semiconductors with a zinc blende structure, the effective potential V can be assumed energy independent, and is equal to $V = E_c$ where $E_c = E_{\Gamma_6}$ is the conduction band (*s*-type symmetry) edge energy [13,14]. Thus, in order that the tunneling condition is satisfied it is necessary that $E = (E_{cA} + E_{cA})$ $(E_{c,B})/2$ and that $\mathbf{M}_A^{-1}(E) = -\mathbf{R}_x \cdot \mathbf{M}_B^{-1}(E) \cdot \mathbf{R}_x$. When the dispersive mass is a scalar we obtain simply $M_A(E) =$ $-M_{R}(E)$; i.e., the effective mass in the two materials must be symmetric at the energy level $E = (E_{c,A} + E_{c,B})/2$. For narrow-gap II-VI semiconductor compounds, to a good approximation the effective mass varies linearly with the energy, so that $M_i(E) = (E - E_{\nu,i})/(2\nu_{P,i}^2), E_{\nu} = E_{\Gamma_8}$ being the valence band (p-type symmetry) edge energy and the velocity v_P is defined by $v_P = \sqrt{E_P/(3m_0)}$, where $E_P = 2P^2 m_0/\hbar^2$, m_0 is the free-electron mass, and P is Kane's parameter [14,15]. Supposing that $v_{P,A} \approx v_{P,B}$, it is simple to check that the tunneling condition reduces to $E_{g,A} = -E_{g,B} E_g = E_c - E_v$ being the band gap energy. Thus, to have "perfect tunneling" one of the materials should have a negative band gap. This can occur in semiconductors with an inverted band structure, such that the conduction band (s-type symmetry) lies below the valence bands (*p*-type symmetry). An example is the II–VI binary compound (semimetal) HgTe for which $E_g =$ -0.3 eV [16]. Let us suppose that the material A is such that $E_{g,A} > 0$ and that the material B (e.g., HgTe) satisfies $E_{g,B} = -E_{g,A}$. We can have two distinct situations: (i) if $0 < (E_{c,A} - E_{c,B})/2 < |E_g|$, or equivalently if $0 < \Lambda/2 <$ $|E_{\rho}|$, the energy level for which the tunneling occurs lies in the band gap of both materials [Fig. 2(a)]; (ii) otherwise the energy level for which the tunneling occurs lies either in the conduction or valence bands of both materials [Fig. 2(b)]. In above, we defined $\Lambda = E_{\nu,B} - E_{\nu,A}$ the valence band offset between the two materials, and used $(E_{c,A} - E_{c,B})/2 = |E_g| - \Lambda/2$. The case (i) may be realized based on heterostructures of $Hg_{1-x}Cd_xTe(A)$ and HgTe (B). For example, if the mole fraction is taken x =0.35 the condition $E_{g,B} = -E_{g,A}$ is expected to be fulfilled with $\Lambda = 0.12$ eV [14,17]. In Ref. [17] we considered the same material combination to predict the supercollimation of electron waves and an extreme anisotropy regime in a semiconductor superlattice exhibiting a highly anisotropic effective mass for electrons. Here, we study instead the strong delocalization of electronic states of a semiconductor heterostructure. The tunneling of electron waves in related heterostructures was recently discussed in Ref. [18], but only for normal incidence.

In the present framework, the heterostructure A-B-A [Fig. 1(b)] can be regarded as a semiconductor quantum well (OW). Mercury telluride-cadmium telluride semiconductor quantum wells have recently received significant attention in the context of the spin Hall effect [19-21]. It was shown that quantum wells with an inverted electronic structure may enable the transport associated with edge states, when the thickness of the well is beyond a certain critical value [19,20]. We calculated the electronic band structure of HgCdTe-HgTe quantum wells using the envelope-function approach [7,22]. Our effective medium theory yields results qualitatively (and also to some extent quantitatively) consistent with those obtained with the Burt-Foreman theory [23,24], which was the basis of the calculations of Ref. [19]. Within our calculations [Fig. 2(c)], the topological phase transition where the electronic states change from a normal to an "inverted" type occurs at the critical thickness $d_c \approx 12a_s = 7.8$ nm with $a_s = 0.65$ nm the lattice constant of the bulk semiconductors. This value of d_c is of the same order ($d_c =$ 6.4 nm) as that predicted in Ref. [19], which gives us confidence in the validity of our approach. In Fig. 2(d) we show the electronic structure of the interfaces states of a QW of Hg_{0.65}Cd_{0.35}Te-HgTe-Hg_{0.65}Cd_{0.35}Te (green lines) with thickness $d = 6a_s$, which corresponds to the above mentioned combination of materials (A-B-A) with $E_{g,2} = -E_{g,1}$ and that may enable "perfect tunneling" at the energy level $E = (E_{c,A} + E_{c,B})/2 \equiv E_0$. As seen, at $E = E_0$ (gray horizontal gridline) the QW does not support



FIG. 2 (color online). (a) Perfect tunneling of an electron wave through a semiconductor heterostructure such that the two materials have symmetric band gap energy $E_{g,2} = -E_{g,1}$ when the valence band offset satisfies $\Lambda < 2|E_g|$. The perfect tunneling occurs for the energy level indicated by the dashed arrows, $E_0 = (E_{c,A} + E_{c,B})/2$. (b) Similar to (a) but for the case $\Lambda > 2|E_g|$. (c) Electronic band structure for the interface states of a quantum well Hg_{0.32}Cd_{0.68}Te-HgTe-Hg_{0.32}Cd_{0.68}Te, qualitatively analogous to Ref. [19]. Black lines: $d = 6a_s$. Green (light gray) lines: $d = 12a_s$. Blue (dark gray) lines: $d = 18a_s$. The solid, dot-dashed, and dashed lines represent the E1 states with even parity, the H1 states with even parity, and the states with odd parity, respectively. (d) Electronic band structure for the interface states of a quantum well Hg_{0.65}Cd_{0.35}Te-HgTe-Hg_{0.65}Cd_{0.35}Te, which may correspond to a combination of materials such that $E_{g,2} = -E_{g,1}$. The gray horizontal gridline represents the energy level E_0 . The black dot-dashed line represents the H1 interface states of a quantum well Hg_{0.65}Cd_{0.35}Te-Hg_{0.90}Cd_{0.10}Te-Hg_{0.65}Cd_{0.35}Te. In all the examples, the energy level E = 0 corresponds to the edge of the valence band (Γ_8) of HgTe.

interface states, and this is qualitatively analogous to Pendry's lens which also does not support guided modes at the frequency where $\varepsilon(\omega_0) = \mu(\omega_0) = -1$.

In the scenario of Fig. 2(a) the energy level $E = E_0$ lies in the band gap of the material A. To show how the QW formed by two complementary materials with symmetric band gap energies may provide a strong delocalization of electronic states, we consider a second QW (Hg_{0.90}Cd_{0.10}Te material C) in the A region (Hg_{0.65}Cd_{0.35}Te) such that the well has thickness $6a_s$. The dispersion of the light-hole (H1) type interface states for this QW is represented in Fig. 2(d) with a dot-dashed black line, showing that at $E = E_0$ the interface states have $k_{\parallel}a_s = 0.14$, where $\mathbf{k}_{\parallel} = (0, k_y, k_z)$ is the in-plane quasimomentum. Let us suppose next that the well *A-B-A* is placed in the vicinity of the well *A-C-A*, such that the spacing between regions *B* and *C* is $l_{QW} = 8a_s$. In these circumstances the two wells are coupled and the confinement of the electronic states can change. The interface states of the coupled QWs at $E = E_0$ can be easily calculated from the knowledge of the interface states of



FIG. 3 (color online). Squared amplitude of the electron wave function (normalized to arbitrary units) for an interface state when the quantum well *A*-*C*-*A* (region *C* has thickness $6a_s$, and the direction of growth is along *x*) is in the vicinity of an "electronic lens" (the region *A*-*B*-*A* delimited by the dot-dashed vertical gridlines). In the region x > 0 the wave function is strongly delocalized from the quantum well. Regions *A*, *B*, and *C* correspond to Hg_{0.65}Cd_{0.35}Te, HgTe, and Hg_{0.90}Cd_{0.10}Te, respectively. The spacing between regions *C* and *B* is $8a_s$. (a) The thickness of the quantum well *B* is $d = 6a_s$. (b) The thickness of the quantum well *B* is $d = 10a_s$. The dot-dashed vertical lines are at a distance d/2 from the region *B*. The wave function has exactly the same value at these virtual planes.

A-C-A, and with the understanding that Bloch modes are transmitted through the region A-B-A with a transmission coefficient $T = e^{-ik_x d}$. Obviously, the electronic states of the well A-C-A are characterized by an imaginary pure k_r $(\gamma_A = -ik_x > 0)$ in material A, which corresponds to the exponential tail of the interface state. Hence, $T = e^{-ik_x d}$ is a real valued growing exponential, and therefore the wave function amplitude is strongly enhanced in the OW A-B-A (Fig. 3). This result is the electronic analogue of the enhancement of evanescent waves in Pendry's lens. In the electronic case, it implies that the lens formed by the two complementary materials with symmetric band gaps provides a strong delocalization of the electronic states associated with the well A-C-A, so that the quantum well A-B-A behaves to some extent as an electron sink at $E = E_0$, and the probability of finding the electron beyond the exit interface of the well A-B-A is strongly enhanced. Counterintuitively, this effect becomes more pronounced when the thickness of the material B is increased, as shown in Figs. 3(a) and 3(b). However, the maximum thickness of the region B is limited by the mean free path length of an electron, which is determined by the temperature, disorder, and defects, among others. Note that because of the "perfect lensing" effect, the profile of the wave function is not disturbed in the region of the well A-C-A, apart from a change of magnitude due to the delocalization of the electronic state. Similar properties can be enunciated for the case of 3D imaging, e.g., for the imaging of a stationary state of a quantum dot at $E = E_0$. Here, we highlighted the imaging of a single Fourier harmonic in order to have our proposal closer to a real-world experiment.

In conclusion, we theoretically derived the general physical principles that may enable the perfect tunneling of stationary states, independent of the angle of incidence, and strong delocalization of interface states in materials with complementary properties, revealing the electronic analogue of the perfect lens effect originally introduced in the context of electromagnetic metamaterials. It can be verified that in the semiconductor and graphene examples considered here (see Ref. [6]), the perfect tunnelling of the propagating stationary states at the interface of the complementary materials is accompanied of a "negative refraction" of the electron velocity, similar to what happens in the case of light waves [1].

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