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Tunable dwell time in gated silicene nanostructures

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ABSTRACT

Residing on the gate-tunable electronic properties of silicene, we have systematically examined the dwell time for quantum tunneling through the single and multiple-gated silicene nanostructures. It is shown that unlike the graphene, superluminal tunneling is observable even at the normal incidence due to the sizeable spin-orbit gap of silicene. Together with its field-tunable bandgap, we show that this superluminal tunneling can be further flexibly switched on and off via electric mean. By simulating the dwell time through the symmetric and asymmetric double barrier structures, it is also shown here that the dwell time displays the distinct dependence on the former and latter barrier profiles. Those observations provide some favorable strategies to experimentally examine and fundamentally understand the time-dependent aspect of tunneling in solid state nanosystems.

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1. Introduction

During the past years, two-dimensional materials with honeycomb lattice have attracted considerable attention [1] due to their exotic Dirac fermion physics and potential applications in atomically nano-electronic devices [2–6]. Among these amazing materials, silicene [7], the monolayer silicon with the low-buckled honeycomb lattice [8], has received particular interest owing to its compatibility with currently integrated technology and the attractive features like field-tunable bandgap and spin-valley locking [9, 10]. Experimentally, besides the synthesis of monolayer and multilayer silicene onto the metallic substrates [11–16], a silicene field effect transistor operating at room temperature has also been reported very recently [17], promising the prospect of silicene-based nanoelectronics.

However, for nanoelectronic devices relying on the tunneling through quantum barriers or wells, the observation of the cutoff frequency or oscillating frequency has brought the urgency to the problem how long it should take a particle to tunnel through the modulated structures, namely tunneling time. To address this problem, many tunneling time definitions have been so far suggested [18,19]. Among these proposals, the dwell time, characterizing the average time of particles spent in the barrier regions, has been regarded as a well-established one [18,19] and extensively employed to understand the time-dependent aspects of tunneling through various solid state nanostructures. Concretely, for the Schrödinger fermions, Winful has theoretically demonstrated the dwell time within a quantum barrier can be related to the scattering phase time (group delay) through a self-interference term [20]. However, for the gapless Dirac fermions, the dwell time could be directly related to the scattering phase time [21,22]. More interestingly, by calculating the dwell time in various graphene barriers [22–26], recent studies have shown that the superluminal or Hartman effect [27] can be engineered in graphene nanostructures by proper strain [25] or magnetic barrier [26] modulations. Thus, considering the appealing properties silicene has, an opening problem is what we could expect the time-dependent aspects of tunneling through silicene-based nanostructures.

In this work, we will focus on the dwell time in single and multiple silicene barriers, which can be further engineered by the nano-gates on top of silicene itself. It is shown here that the superluminal tunneling can be flexibly switched on/off in silicene-based structures by the top gate modulation, and for the double barrier structure, each barrier has different functions in engineering the dwell time or superluminal tunneling in the concerned silicene nanostructures, thus providing several beneficial strategies to experimentally study and fundamentally understand the tunneling time in solid state nanosystems.

2. Model and equation

Our considered structure is schematically depicted in Fig. 1(a), where a sheet of silicene synthesized onto the bottom substrate is locally modulated by the top gate arrays with a thin dielectric spacer. Each top gate has width L and separates from its adjacent counterparts with a distance w. Thus, under the gate bias

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Fig. 1. (Color online.) (a) Schematic sketch of our model structure and (b) the typical potential profiles for the illustrative dual-gated configuration.

modulation, the local potential profiles could be efficiently engineered, forming further various silicene nano-domains to modulate the transport properties of Dirac fermions. Illustratively, assuming the uniform gate-modulation, Fig. 1(b) depicts the general potential profiles for the top dual gate structure. Remarkably, contrary to graphene, silicene acquires a sizeable spin–orbit gap, and once turning on the electrostatic potential (U) and local field (Δ_z) modulation together, different band alignments could be engineered [28], making the concerned structure can systematically mimic both type-I and type-II band profiles as frequently observed in the conventional semiconductor heterostructures. In the vicinity of the Dirac point (K and K'), the electronic properties for our considered structure can be well described by the following low-energy effective Hamiltonian [29,30], reading

$$H = \begin{bmatrix} -\eta \sigma \Delta_{so} + \Delta_z(x) + U(x) & \hbar v_f(k_x + i\eta k_y) \\ \hbar v_f(k_x - i\eta k_y) & \eta \sigma \Delta_{so} - \Delta_z(x) + U(x) \end{bmatrix}$$
(1)

with $v_f = 5.5 \times 10^5$ m/s the Fermi velocity, \hbar the reduced Planck constant, k_x/k_y the longitudinal/transverse wave vector, $\Delta_{so} = 3.9$ meV the intrinsic spin–orbit interaction, $\sigma = \pm 1$ with plus/minus for the spin-up/down orientation electron, $\eta = \pm 1$ with plus/minus for the K/K' valley, Δ_z the on-site potential difference between the A- and B-sublattice, which can be efficiently tuned by the local electric field [31–33], and *U* the gate-biased electrostatic potential. For a uniform modulation, both Δ_z and *U* have a finite value beneath the gates, while zero for the others, including the terminals and the domain uncovered by the top gates. Thus, because of the translation invariant along the *y*-direction, the transverse momentum k_y is conserved during the tunneling process. By solving the above Hamiltonian for our concerned system, the energy dispersion could be further derived as

$$E = U \pm \sqrt{(\hbar \nu_f k)^2 + (\eta \sigma \Delta_{so} - \Delta_z)^2}$$
⁽²⁾

with $k^2 = k_x^2 + k_y^2$ and the corresponding eigenspinors wave function ϕ yielding

$$\phi_{\pm} = \frac{1}{\sqrt{2(E-U)E_N}} \begin{bmatrix} \hbar v_f (\pm k_x + i\eta k_y) \\ E_N \end{bmatrix} e^{\pm ik_x x + ik_y y}$$
(3)

where the subscript with plus/minus denotes the forward/backward state and $E_N = E - U + \eta \sigma \Delta_{so} - \Delta_z$. Here as an illustrative example, the algebra procedures for the shown dual-gate configuration are briefly summarized. Specifically, we consider a beam of Dirac fermions impinges onto the modulated structure from left to right with energy *E* and incident angle θ . Thus, within the incident terminal (x < 0), the resulting wave-function φ_{in} can be written as

$$\rho_{in} = \frac{e^{ik_x^{in}x + ik_y y}}{\sqrt{2E(E + \eta\sigma\Delta_{so})}} \begin{bmatrix} \hbar v_f(k_x^{in} + i\eta k_y) \\ E + \eta\sigma\Delta_{so} \end{bmatrix} \\
+ \frac{re^{-ik_x^{in}x + ik_y y}}{\sqrt{2E(E + \eta\sigma\Delta_{so})}} \begin{bmatrix} \hbar v_f(-k_x^{in} + i\eta k_y) \\ E + \eta\sigma\Delta_{so} \end{bmatrix}$$
(4)

where *r* is the reflection coefficient, $k_x^{in} = k \cdot \cos \theta$, and $k_y = k \cdot \sin \theta$ with $k = \sqrt{E^2 - \Delta_{so}^2} / \hbar v_F$.

For the output terminal (x > 2d + w), the corresponding wavefunction can be written as

$$\varphi_{0} = \frac{te^{ik_{x}^{0}x + ik_{y}y}}{\sqrt{2E(E + \eta\sigma\Delta_{so})}} \begin{bmatrix} \hbar\nu_{f}(k_{x}^{0} + i\eta k_{y}) \\ E + \eta\sigma\Delta_{so} \end{bmatrix}$$
(5)

with *t* the transmission coefficient and $k_x^0 = \sqrt{E^2 - \Delta_{so}^2 - (\hbar v_F k_y)^2} / \hbar v_F$.

Within the rest modulated regions, the wave-function in each domain can be unifiedly expressed as

$$\varphi_{j} = a_{j}e^{iq_{x}^{j}x+ik_{y}y} \begin{bmatrix} \hbar\nu_{f}(q_{x}^{j}+i\eta k_{y}) \\ E_{N}^{j} \end{bmatrix} + b_{j}e^{-iq_{x}^{j}x+ik_{y}y} \begin{bmatrix} \hbar\nu_{f}(-q_{x}^{j}+i\eta k_{y}) \\ E_{N}^{j} \end{bmatrix}$$
(6)

where j = 1, 2, 3 numbers orderly the specific domain from left to right, $a_j(b_j)$ is the unknown coefficient,

$$q_x^j = \sqrt{(E - U^j)^2 - (\eta \sigma \Delta_{so} - \Delta_z^j)^2 - (\hbar v_F k_y)^2} / \hbar v_F,$$

and $E_N^j = E - U^j + \eta \sigma \Delta_{so} - \Delta_z^j.$
Applying the wave-function continuity requirement at t

Applying the wave-function continuity requirement at the interfaces of each domain and following the standard transfer matrix method, one can directly relate the transmission coefficient t with those at the incident terminal through a total transfer matrix M, yielding

$$\begin{bmatrix} 1\\r \end{bmatrix} = M \begin{bmatrix} t\\0 \end{bmatrix}$$
(7)

From the above equation, t can be further determined as

$$t = 1/M_{11}$$
 (8)

Thus, other unknown coefficients can be explicitly related with t, and the concerned transmission probability T can thus be determined as

$$T = \frac{k^o}{k^{in}} |t|^2 \tag{9}$$

In this context, the concerned dwell time τ_d defined as the integrated probability density within the modulated regions can be calculated from the following equation [19,20], reading

$$\tau_d = \int_0^L \frac{|\varphi_M(x, y)|^2}{J_{in}} dx$$
(10)

where *L* is the total length of modulated regions, $J_{in} = v_F \times \sqrt{1 - (\Delta_{so}/E)^2} \cos \theta$ is the flux of the incident carriers, and φ_M denotes the wave-function within the modulated regions.

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