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Generation of valley pump currents in silicene*

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We propose a workable scheme for generating a bulk valley pump current in a silicene-based device which consists of two pumping regions characterized by time-dependent strain and staggered potentials, respectively. In a one-dimension model, we show that a pure valley current can be generated, in which the two valley currents have the same magnitude but flow in opposite directions. Besides, the pumped valley current is quantized and maximized when the Fermi energy of the system locates in the bandgap opened by the two pumping potentials. Furthermore, the valley current can be finely controlled by tuning the device parameters. Our results are useful for the development of valleytronic devices based on two-dimensional materials.

Keywords: valley currents, charge pump, quantization, silicene

PACS: 72.25.Dc, 72.80.Vp, 73.20.At, 85.75.–d **DOI:** 10.1088/1674-1056/28/1/017204

1. Introduction

The discovery and synthesis of new two-dimensional (2D) materials with hexagonal lattice structures, such as silicene,[1–6] have greatly advanced the study of quantum physics, and can help overcome the difficulties associated with graphene to enable future applications in the next-generation electronic devices.[7–22] Silicene, a silicon analogue of graphene, is a monolayer of silicon atoms instead of carbon atoms assembling in a honeycomb lattice and has been extensively explored both theoretically[23–26] and experimentally.[27,28] Silicene inherits some properties from graphene, such as electrons in silicene are linearly dispersed within the low-energy regime. Besides, silicene introduces advanced and distinguishing features thanks to its prominent buckled structure that the two inequivalent sublattices A and B are not coplanar, which allows us to adjust the Dirac mass by a perpendicular electric field (E-field)[25,29–32] and brings some unique electronic transport properties.[18,33–35] Therefore, the manipulation of Dirac electrons in the silicene systems will also be of great importance.

It is worthy of note that in the early years, those works on the physics of valleytronics[36–39] have aroused considerable interest among researchers. The key issue in the exploitation of valley degree of freedom of electrons is the generation of pure valley current, which consists of two oppositely flowing distinct currents originated from the two inequivalent conical (Dirac) points K and K' valleys in Brillouin zone,[30,40–63] resembling the pure spin current.[7,8,24,63–83]

On the other hand, quantum pumping[58,84–90] is a useful technique which can generate dc currents without bias voltage. It uses two pumping parameters as ac signals to modify the electron transport of nanostructures and further alter the scattering characteristics of the device. When two ac signals are out of phase and their periods are longer than the time required for the electrons to traverse the device, a nonzero pump current is generated.[86,91] Recently, Jiang *et al*. proposed to generate a pure valley current based on the quantum pumping effect by employing the lattice strain.[40] However, that approach is technically complicated. In this regard, it is extremely desirable to have an alternative, which minimizes the technical and experimental requirements by using the time-dependent strain and E-field to directly generate the valley pump currents.

In this paper, we propose an uncomplicated method to generate pure valley pump currents in a silicene-based two-parameter pump device, in which the pumping sources are the time-dependent lattice strain[92,93] and staggered potential generated by the time-dependent lattice deformation and perpendicular E-field, respectively. It is found that the strain and staggered potential are necessary for breaking the degeneracy of the K and K' valleys and leading to a pure valley pump current. Due to the quantum interference effect, the valley pumped current can be modulated by controlling the pump parameters. Besides, when the Fermi energy lies in the bandgap opened by the pumping potentials, the pumped currents are maximized and quantized.

2. Model

In this work, we consider a pump device based on silicene as schematically shown in Fig. 1. The silicene sheet is in the xy plane, in the spirit of an adiabatic quantum pump, two pumping regions characterized by two oscillating pumping potentials $A(t)$ and $\Delta(t) = E_z(t)l$ generated from the time-

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dependent longitudinal strain and perpendicular E-field $E_z(t)$ respectively are introduced, with l being the buckling height between sublattices A and B.[95] The whole pump device is connected with the outside by the left (L) and right (R) leads without any bias. The lengths of both pumping regions are L along the current direction (the x axis). The transverse direction (the y axis) is assumed homogeneous so the system observes translational symmetry.

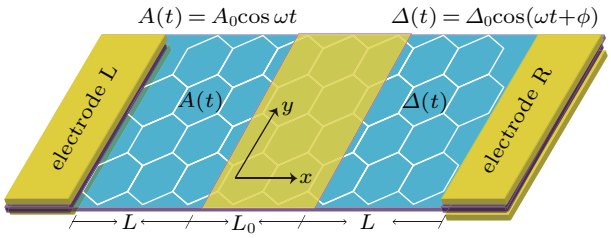


Fig. 1. Schematic of the proposed silicene-based two-terminal pump device. The silicene sheet is in the xy plane; the two pumping sources, with L in length, are the strain $A=A_0\cos\omega t$ and staggered potential $\Delta=\Delta_0\cos(\omega t+\phi)$ with a phase lag ϕ and a distance L_0 between them. The device is connected to electrodes by the left (L) and right (R) leads, the pumped current is assumed along the x axis.

We shall analyze the character of the valley pump current in the adiabatic pumping process.[94] To this end, we employ the low-energy continuum Hamiltonian[20,59–63,95,96] of silicene, then we solve the time-dependent formulation using scattering matrix. The silicene system can be described by the following continuum model:

$$\mathcal{H}=\hbar v_{\mathrm{F}}(\sigma_x k_x+\eta k_y\sigma_y)+V_0+\eta A(t)\sigma_y\Theta_1+\Delta(t)\sigma_z\Theta_2, \quad (1)$$

where $\sigma_{x,y,z}$ is the Pauli matrix acting on the pseudospin space associated with the A and B sublattices, $\Theta_1=\Theta(x)\Theta(L-x)$ and $\Theta_2=\Theta(x-L_0-L)\Theta(2L+L_0-x)$ with $\Theta(x)$ being the Heaviside step function. The first term describes the pristine silicene, $k_{x,y}$ is the x,y-component momentum of particles and $\eta=\pm1$ is the valley index denoting the K or K' valley. The second term V_0 denotes the local controllable potential, which can be modulated by an external voltage gate and is assumed in the central region in our model. The last two terms denote homogeneous finite-length L pumping regions: $A=A_0\cos\omega t$ and $\Delta=\Delta_0\cos(\omega t+\phi)$ with the pumping strengths A_0 and Δ_0, respectively, where ω is the pumping frequency, and ϕ is the pumping phase shift. They break the inversion symmetry of silicene and open a bandgap of Dirac electrons, which turns silicene into a quantum valley Hall insulator (QVHI). Here, A originates from the elastic deformation of the silicene lattice;[92,93] Δ arises from the vertical E-field applied onto the sheet. The two pumping potentials with opposite signs produce opposite Chern numbers,[97] therefore induce a topological interface state (TIS) between them, and finally produce quantized pumping currents[98] when the Fermi energy E situates in the bandgap.

In the zero-temperature and adiabatic limit, the pumped current can be evaluated directly by adopting the BTP formula[99]

$$I_{\alpha\pm}=\frac{\mathrm{i}e}{2\pi T}\int_0^T \mathrm{d}t\mathrm{Tr}\left(\frac{\partial\mathcal{S}_\pm}{\partial t}\mathcal{S}_\pm^*\right)_{\alpha\alpha}, \quad (2)$$

where $T=2\pi/\omega$ is the pump cycle, $\mathcal{S}_{\alpha\beta}$ is the instantaneous scattering matrix with $\alpha(\beta)=$ L, R being the L/R lead index, and is often expressed as

$$\mathcal{S}_\pm=\begin{pmatrix}\tilde{r}_\pm & \tilde{t}'_\pm\\ \tilde{t}_\pm & \tilde{r}'_\pm\end{pmatrix}. \quad (3)$$

Here $\tilde{r}_\pm$ ($\tilde{r}'_\pm$) and $\tilde{t}_\pm$ ($\tilde{t}'_\pm$) are the left (right) reflection and transmission matrices, respectively. The trace runs over the transverse modes and $\pm=K$ (K') is the valley index. The adiabatic limit renders the transverse momentum k_y conserved in the instantaneous scattering process.

With the aim of figuring out the scattering coefficients, the following combining method is preferred. The formulae of two required coefficients, $r_\pm$ and $t'_\pm$, in two individual scattering events at A and Δ potentials are

$$\tilde{r}_\pm=r_1+\frac{\mathrm{e}^{\mathrm{i}\varphi_\pm}t_1^2r_2}{1-r_1r_2\mathrm{e}^{\mathrm{i}\varphi_\pm}}, \quad (4)$$

$$\tilde{t}'_\pm=\frac{t_1t_2}{1-r_1r_2\mathrm{e}^{\mathrm{i}\varphi_\pm}}, \quad (5)$$

with the dynamic phase of electrons passing through the central region

$$\varphi_\pm=k_\pm L_0=L_0\sqrt{(E-V_0)^2-k_y^2}, \quad (6)$$

where r_i and t_i ($i=1,2$) are the reflection and transmission amplitudes of the i-th pumping potential, respectively. For instance, r_1 and t_1 can be solved by exploiting the scattering process which describes the first pumping potential A,

$$\Psi(x)=\begin{cases}\begin{pmatrix}1\\1\end{pmatrix}\mathrm{e}^{\mathrm{i}k_xx+\mathrm{i}k_yy}+r_1\begin{pmatrix}1\\-1\end{pmatrix}\mathrm{e}^{-\mathrm{i}k_xx+\mathrm{i}k_yy}, & x<0,\\ a\begin{pmatrix}k_x-\mathrm{i}A\\E\end{pmatrix}\mathrm{e}^{\mathrm{i}\kappa_xx+\mathrm{i}k_yy}+b\begin{pmatrix}-k_x-\mathrm{i}A\\E\end{pmatrix}\mathrm{e}^{-\mathrm{i}\kappa_xx+\mathrm{i}k_yy}, & 0<x<L,\\ t_1\begin{pmatrix}1\\1\end{pmatrix}\mathrm{e}^{\mathrm{i}k_xx+\mathrm{i}k_yy}, & x>L.\end{cases} \quad (7)$$

The above three wavefunctions are respectively in the first three regions on the left of the device. The momenta of electrons in the normal and potential regions are given by $k_x = \sqrt{E^2 - k_y^2}$ and $\kappa_x = \sqrt{E^2 - k_y^2 - A^2}$, respectively ($\hbar v_F = 1$). r_2 and t_2 at the second pumping potential Δ can also be obtained in a similar way. r_2' and t_2' can be determined afterwards by considering the injection from the right, conjugate to the process of Eq. (7).

3. Results

Armed with the groundwork above, we can straightforwardly calculate the valley-resolved pumped current $I_{LK(K')}$ flowing through the L lead of the proposed pump device according to Eq. (3). Since the quantized pumped currents are the focus, which come up when the Fermi energy situates in the bandgap opened by A and Δ, the transverse momentum k_y does not quantitatively affect the results,[98] we can just consider a pure one-dimensional case, $k_y = 0$.

Firstly, we plot the valley-resolved pumped current $I_{LK(K')}$ as a function of the pumping phase ϕ in Fig. 2. One can see that the pumped currents for the two valleys have the same magnitude but opposite directions, this implies that a pure valley current can be pumped.

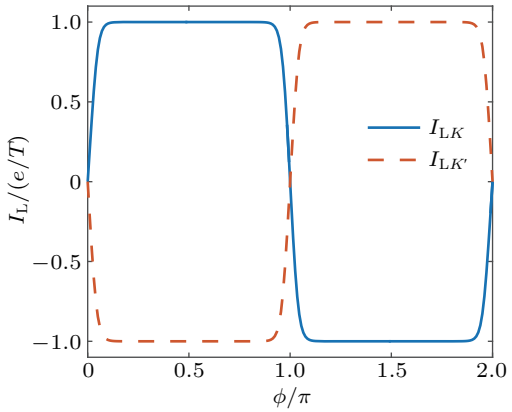


Fig. 2. Valley-resolved pumped current $I_{LK(K')}$ as a function of ϕ. Other parameters are $E = 0.01$ eV, $A_0 = 1$ eV, $\Delta_0 = 1$ eV, $L_0 = 0$, and $L = 10a$ with a being the lattice constant.

Most importantly, $I_{LK(K')}$ deviates from the supposed sine-function behavior $I \sim \sin\phi$ of an adiabatic quantum parameter pump because the obtained pumped current is quantized as the Fermi energy $|E| \ll A_0$ and Δ_0. Therefore, they finally show $I_{LK(K')} = \pm e/T$. The physics inside the quantization is the TIS[98] forming between two time-evolving pumping potentials. Either strain or staggered potential will generate a QVHI phase in the pumping region,[18] but this phase has no boundary or edge state. Thus the interface state with zero energy will emerge in the joint undoubtedly when $\mathrm{sgn}(A) = -\mathrm{sgn}(\Delta)$. This TIS, together with the Fermi energy situated in the bandgap, proves the quantization of the valley pump current.

Here comes to mind that the pumping action is a quantum interference effect in nature, the outcomes can be inevitably tuned by the dynamic phase of electrons φ[83] in Eq. (6). Thus, one can also utilize either Fermi energy E or the length L_0 of the central region to control the pumping output.

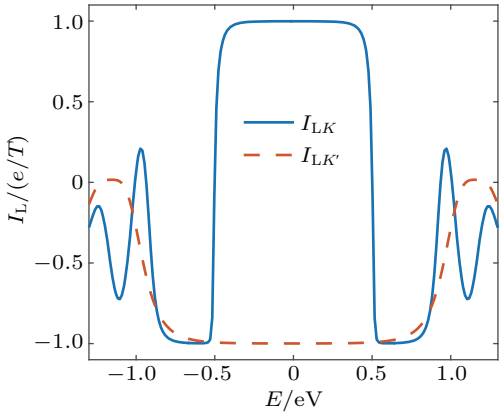


Fig. 3. Valley-resolved pumped current $I_{LK(K')}$ as a function of the Fermi energy E. The lengths of the pump regions are $L = 6a$. Other parameters are $A_0 = 1$ eV, $\Delta_0 = 1$ eV, and $L_0 = 0$.

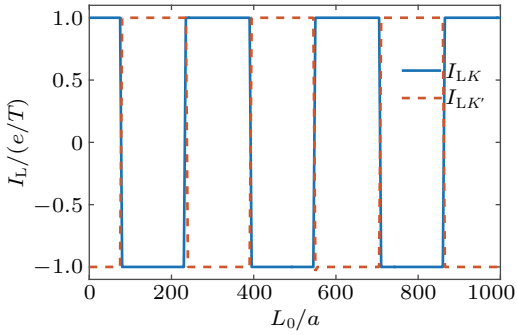


Fig. 4. Valley-resolved pumped current $I_{LK(K')}$ as a function of the length of the central normal region L_0. The lengths of the pump regions are $L = 10a$. Other parameters are $E = 0.01$ eV, $A_0 = 1$ eV, and $\Delta_0 = 1$ eV.

Then we present the valley currents as a function of E and L_0 in Figs. 3 and 4, respectively. They both validate that the pumping currents are maximized and quantized when the Fermi energy E lies in the bandgap. It is also easy to get that the symmetry property of the structure plays an important role in obtaining the pure valley current in the whole energy region. When the two pumping potentials are symmetric about the central line of the structure, the Hamiltonians of the two valleys deliver the relationship $I_K = -I_{K'}$. So that one can obtain nonzero valley current[40] $I_v = I_K - I_{K'}$. Similar to Fig. 2, I_L exhibits an abrupt reversal between the two quantized values $\pm e/T$ in Fig. 4. They confirm the effect of the dynamic phase of electrons in modulating I_L.[98]

Note that it is not strange to achieve valley pumped currents in devices, but the proposed model can yield an optimal pumping effect of valley pump currents, i.e., the valley pumped current is maximized for each transport model. Moreover, as discussed in Ref. [98], a larger transverse momentum

k_y makes the propagating energy smaller and more likely to be located in the bandgap, so the quantization of pumping currents is more prone to appear. Here, we have discussed the ideal valley pumped currents in a silicene-based device by using the time-dependent elastic deformation and E-field which induce strain and staggered potential, respectively. Furthermore, these results also hold true in devices based on other 2D materials. However, the transport direction is crucial since the bandgap which is necessary for the quantized pump currents cannot exist along all directions. This is also the reason why we consider a one-dimensional pump device, only the perpendicular incident electrons encounter the energy gap due to the lattice deformation.

4. Conclusion

In summary, we have proposed to generate pure valley pump currents in a silicene-based device by cyclic modulation of time-dependent strain and staggered potential. We calculated the pumped currents in the one-dimensional case by setting the transverse momentum to zero and found them quantized when the Fermi energy resides in the energy gap opened by the pumping potentials. Furthermore, a pure valley pump current can be obtained by tuning the relevant parameters such as the phase lag and the dynamic phase of electrons. Our findings are helpful for the generation of pure valley pump currents in the Dirac-electron systems, the proposed structure can be applied in the realization of silicene valleytronic devices.

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