Strained graphene based highly efficient quantum heat engine operating at maximum power

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A strained graphene monolayer is shown to operate as a highly efficient quantum heat engine delivering maximum power. The efficiency and power of the proposed device exceeds that of recent proposals. The reason for these excellent characteristics is that strain enables complete valley separation in transmittance through the device, implying that increasing strain leads to very high Seebeck coefficient as well as lower conductance. In addition, since time-reversal symmetry is unbroken in our system, the proposed strained graphene quantum heat engine can also act as a high performance refrigerator.

I. INTRODUCTION

Quantum heat engines (QHE) have twin purposes to act as highly efficient heat engine enabled by quantum principles and also to act as a conduit for excess heat therein lies their appeal. In this work we probe the thermo-electric properties of an open strained graphene system and show its action as a very efficient quantum heat engine (QHE). Earlier, a closed strained graphene system has been shown to operate as a QHE. A closed system differs from an open system in that no transport of heat or charge current is involved in the operation of such a closed heat engine. Closed heat engines operate on the principle that the outside environment is almost decoupled from the system. In the quantum regime most of these closed QHE operate in the single particle regime, meaning these are more of theoretical constructs than with wide experimental applicability. Open system QHE on the other hand are enabled due to charge and heat transport, thus these are actively coupled to the environment and thereby with more experimental and possible commercial applications.

II. THEORY

Our aim in this work is to design an extremely efficient QHE which operates at full power using a strained graphene system. To do this we calculate the thermoelectric properties of our system in the linear transport regime, wherein electric and heat currents are linearly proportional to the applied biases be it electric or thermal. In a thermoelectric system temperature difference across the system work in tandem to operationalise it. The linear dependencies can be expressed as follows:

\[
\left( \begin{array}{c}
    j_x \\
    j_y
\end{array} \right) = \left( \begin{array}{cc}
    L_{11} & L_{12} \\
    L_{21} & L_{22}
\end{array} \right) \left( \begin{array}{c}
    \Delta T \\
    \Delta E
\end{array} \right)
\]

where \( j_x \) and \( j_y \) are the electric and heat currents respectively, \( L_{ij} \) with \( i,j \in \{1,2\} \) represents Onsager coefficients for a two terminal thermo-electric system. The Seebeck coefficient is defined as the electric response due to the finite temperature difference across the system. On the other hand, the Peltier coefficient \( P \) is defined as the heat current generated due to the applied bias voltage \( \Delta E \) across the system. They are expressed as follows:

\[
S = -\frac{L_{12}}{L_{11}}, \quad \text{and} \quad P = \frac{L_{21}}{L_{11}}
\]

The Onsager co-efficient matrix in Eq. (1), which relates the electric and heat currents to the temperature differences and applied electric bias, can be rewritten as follows:

\[
\left( \begin{array}{cc}
    L_{11} & L_{12} \\
    L_{21} & L_{22}
\end{array} \right) = \left( \begin{array}{cc}
    L^0 \\
    L^1 / e
\end{array} \right) \left( \begin{array}{cc}
    \Delta E / eT \\
    \Delta T
\end{array} \right)
\]

wherein,

\[
L^\alpha = G_0 \int_{-\pi/2}^{\pi/2} d\phi \cos \phi \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{\partial f}{\partial \varepsilon} \right) \frac{|\varepsilon|}{\hbar v_f} (\varepsilon - \mu) T(\varepsilon, \phi)
\]

here \( G_0 = (e^2/h)(W/\pi^2) \), \( L^0 = G \) is conductance of system with sample width \( W \), \( \phi \) is the angle at which the electron is
incident, $\varepsilon$ is the energy of the electron, $f$ is the Fermi-Dirac distribution, $\mu$ is the Fermi energy and $T(\varepsilon, \phi)$ is the transmission probability for electrons through strained graphene. To calculate the Onsager coefficients $L^{ij}$ in Eq. (1), we need the transmission probability $T(\varepsilon, \phi)$. After calculating the Onsager coefficients $L^{ij}$ in Eq. (1), maximal efficiency and power can be determined, as follows. The output power, defined as:

$$\mathcal{P} = j^*E = (L^{11}E + L^{12}A^T)E$$

is maximized by $\frac{d\mathcal{P}}{dE} = 0$, at $E = -\frac{L^{11}}{2L^{12}}\Delta T$, which gives maximum power as:

$$P_{\text{max}} = \frac{1}{4}(\frac{L^{12}}{L^{11}})^2(\Delta T)^2 = \frac{1}{4}S^2G(\Delta T)^2$$

The efficiency at maximum power is defined as the ratio of maximum power to the heat current transported and is derived to be:

$$\eta \left( P_{\text{max}} \right) = \frac{\eta_c}{\frac{2}{2L^{11}L^{22} - L^{12}L^{21}}} = \frac{\eta_c}{2 + GS^2T/\kappa}$$

Similarly, efficiency $\eta$ becomes:

$$\eta = \frac{P}{\mathcal{P}} = \frac{(L^{11}E + L^{12}A^T)E}{(L^{21}E + L^{22}A^T)} = \frac{-E - S\Delta T}{(TS - \frac{2}{2} + TS^2\Delta T)}$$

To calculate maximal efficiency we need to find the relation between $E$ and $\Delta T$, substituting $\frac{d\mathcal{P}}{dE} = 0$ in Eq. (6), with the condition $j^* > 0$, gives:

$$E = \frac{L^{22}}{L^{21}}(-1 + \sqrt{\frac{L^{11}L^{22} - L^{12}L^{21}}{L^{11}L^{22}}})\Delta T$$

and,

$$\eta_{\text{max}} = \eta_c \sqrt{\Delta T + 1 - \frac{1}{\sqrt{\Delta T}}}$$

wherein $\eta_c$ is the Carnot efficiency defined by $\Delta T$ and $ZT$ is the figure of merit, a dimensionless quantity, defined as:

$$ZT = \frac{GS^2T}{\kappa}$$

### III. MODEL

#### A. Hamiltonian

Graphene is a 2D Carbon allotrope with honeycomb lattice structure which consists of two triangular sublattices A and B. To design our system we apply an uniaxial mechanical strain to the monolayer graphene sheet lying in the x-y plane between $x = 0$ and $x = a$. A potential bias is applied at contact 1 with a finite temperature difference between the two contacts 1 and 2.

The corresponding set up is shown in Fig. 1. In Fig. 1, a general two terminal thermodynamic model is shown to operate between two temperatures $T_1 > T_2$ and a bias $\Delta V = V_1 - V_2$. At steady state, a steady heat and electric current, $j^* = j^*$ flow between these two reservoirs. If $j^* > 0$ and output (as defined in Eq. (5)) power $> 0$ then it is a QHE and if $j^* < 0$ and output power $< 0$ then it acts as a refrigerator.

In Landau gauge, the strain can be expressed as a pseudo magnetic vector potential $A = (0, z, A_z)$, where '+' and '-' signs are for $K$ and $K'$ valley respectively. This system is described by the Hamiltonian, which is given for $K$ and $K'$ valleys as:

$$\mathcal{H}_K = h\nu_f(\sigma - s) \quad \mathcal{H}_{K'} = -h\nu_f^\sigma(\sigma - s)$$

where $s = \frac{\Delta u}{h
u_f}[\Theta(x) - \Theta(x - a)]$ is the strain, $\sigma = (\sigma_x, \sigma_y)$ are the Pauli matrices operating on the sublattices A and B with $\sigma^*$ being the complex conjugate, $k = (k_x, k_y)$ is the 2D wave vector, $\Theta$ being the step function and $v_f$ the Fermi velocity. Solving the Hamiltonian in Eq. (12), we can write the wave equation for $K$ valley as:

$$h\nu_f(-i\partial_x - iy - is)\psi_B = E\psi_A$$

$$h\nu_f(-i\partial_x + iy + is)\psi_A = E\psi_B$$

In the next subsection we will solve Eq. (14) to calculate the transmission $T(\varepsilon, \phi)$ for ballistic transport in monolayer graphene with uniaxial strain.

### B. Wave function and Boundary conditions

Let us consider an electron with energy $\varepsilon$ incident on the interface between region 1 and 2 with angle $\phi$, which can reflect or transmit depending on its energy and angle of incidence. Here, we have three well defined regions-normal graphene $\varepsilon < 0$, strained graphene between $x = 0$ and $x = a$ and again normal graphene for $x > a$. The wave functions for the three regions for A and B sublattices in $K$ valley are given below.

For, $x < 0$:

$$\begin{bmatrix} \psi_A^1(x, y) \\ \psi_B^1(x, y) \end{bmatrix} = \begin{bmatrix} (e^{ik_x x + re^{ik_y y}}) \\ (e^{ik_x x - i(e^{ik_y y} - 1)}) \end{bmatrix} e^{ik_y y}$$

in region $0 < x < a$:

$$\begin{bmatrix} \psi_A^2(x, y) \\ \psi_B^2(x, y) \end{bmatrix} = \begin{bmatrix} (ae^{iq_x x} + be^{-iq_x x}) \\ (ae^{iq_x x + i\theta} - be^{-iq_x x - i\theta}) \end{bmatrix} e^{ik_y y}$$

and for $x > a$:

$$\begin{bmatrix} \psi_A^3(x, y) \\ \psi_B^3(x, y) \end{bmatrix} = \begin{bmatrix} te^{ik_x x} \\ te^{ik_x x + i\theta} \end{bmatrix} e^{ik_y y}$$

where $q_x = \sqrt{(\varepsilon/h\nu_f)^2 - (k_y - s)^2}$ is the x component of momentum wave vector inside the strained region. In the normal regions $q_x$ is replaced with $k_x$ and $k_x^2 + k_y^2 = (\varepsilon/h\nu_f)^2$ wherein $k_x = (\varepsilon/h\nu_f)\cos \phi$ and $k_y = (\varepsilon/h\nu_f)\sin \phi$. In the strained region $q_x = (\varepsilon/h\nu_f)\cos \theta$ and $k_x - s = (\varepsilon/h\nu_f)\sin \theta, \theta$ being the refraction angle in the strained region as shown in Fig. 1 (bottom) and also satisfies $\tan \theta = (k_y - s) / q_x$. To solve Eq. (14) for
the wave functions in Eqs. (15-17) we impose following boundary conditions-

\[ \psi^2_B(x = 0) = \psi^1_B(x = 0), \quad \psi^2_A(x = 0) = \psi^1_A(x = 0) \quad (18) \]

and at \( x = a \),

\[ \psi^2_A(x = a) = \psi^3_A(x = a), \quad \psi^2_B(x = a) = \psi^3_B(x = a). \quad (19) \]

Solving Eqs. (18-19) we get the transmission probability for \( K \) valley as-

\[ T(\epsilon, \phi) = \frac{1}{\cos^2[q_sL] + \sin^2[q_sL](\frac{1-\sin[\phi]\sin[\phi]}{\cos[\phi]\cos[\phi]})^2} \quad (20) \]

Finally from the Hamiltonian for \( K' \) valley as in Eq. (13) and imposing boundary conditions similar to that for \( K \) valley and then replacing \( \phi \to -\phi \), \( s \to -s \) we get the transmission probability for \( K' \) valley. The total conduction then is sum of both \( K \) and \( K' \) valley conductances. It so turns out that although transmission \( T(\epsilon, \phi) \) differs in \( K \) and \( K' \) valley, when integrated over \( \phi' \) this differences disappear. Thus total conductance \( G \) is the twice that of \( K \) valley conductance.

### IV. RESULTS AND DISCUSSION

Our aim as defined in the introduction was to design an efficient QHE operating at maximum power via strained graphene. The generated power should be comparable to or better than other QHE’s based on quantum Hall effect\(^{[10]}\), chaotic cavities\(^{[9]}\), etc. To generate maximum power the system should have a large Seebeck coefficient \( (S) \) with a large electrical conductance \( (G) \), as power is proportional to the \( S^2G \), see Eq. (6).

Increasing strain reduces the electrical conductance, see Fig. 2, but increases the Seebeck coefficient, as in Fig. 3. As strain increases the transmittance of electrons through strained graphene decreases, thus reducing the electrical conductance. From Fig. 2, we see that increasing strain opens a gap in the conduction, not a band gap, it is due to the shift of the Dirac cones by the strain in the Brillouin zone. A real energy band gap opens for a strain beyond 20 percent (540 meV) in pristine graphene\(^{[8]}\), so we will restrict ourselves only to a maximum of 15 percent strain (400 meV). A sign change seen in Fig. 3, for the Seebeck co-efficient near the charge neutrality point (CNP), is due to switching between hole and electron carriers. The first peak, close to the CNP, is due to the imbalance between electron and hole contributions to the thermo-electric co-efficient \( L \), and is present even at zero strain. This peak dies at a distance from the CNP. The origin of the second peak in the Seebeck co-efficient (blue line in Fig. 3) is due to the applied strain. As a result of this strain, transmission becomes a function of the Fermi energy and gives rise to a large Seebeck co-efficient, which leads to large power with finite efficiency.

At lower levels of strain \( (s = 50 \text{ meV}) \) our proposed QHE can exhibit maximum power, i.e., \( 0.2 \frac{(k_b \Delta T)^2}{h} = 0.057 \text{ pico Watt} \) at 30 K for 40 nm strained region, with \( \Delta T = 1K \), see Figs. 4 and 5. This is more than what is seen in two and three terminal quantum Hall heat engines operating at maximum power\(^{[10]}\), The efficiency at maximum power \( \eta(P_{\text{max}}) \) is \( 0.1 \eta_c \), which is also good enough as compared to the other QHE’s, see Fig. 6. Efficiency at maximum power can also be raised to more than...
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Figure 5. Maximum Power ($P_{\text{max}}$) at temperature $T = 30K$, for varying strains and Fermi energy $E_f$ with length $L = 40nm$, and width $W = 20nm$ of strained region.

Figure 6. Efficiency at maximum power at temperature $T = 30K$ with strain $s = 50meV$, width of strained region $W = 20nm$.

Figure 7. Efficiency at maximum power $\eta(P_{\text{max}})$ at temperature $T = 30K$ with width $W = 20nm$ and $L = 40nm$ of strained region.

Figure 8. (a) Maximum Efficiency $\eta_{\text{max}}$ and $\eta(P_{\text{max}})$ at 30K, for Fermi velocity $v_f = 10^6 m/s$ and (b) Maximum Efficiency $\eta_{\text{max}}$ and $\eta(P_{\text{max}})$ at temperature 30K and Fermi velocity $v_f = 6 \times 10^5 m/s$ with width $W = 20nm$ of strained region, other parameters are mentioned in plots itself.

0.4 $\eta_c$, as in Fig. 7, but then maximum power $P_{\text{max}}$ reduces to less than 0.03 $(k_b \Delta T)^2/h$. This is because maximum power generated in the QHE depends on both Seeback co-efficient and electrical conductance, see Eq. (6), and these two factors so conspire to reduce the maximum power. However, the overall efficiency at maximum power again though dependent on Seeback co-efficient ($\eta_c$), conductance $G$ and thermal conductance $\kappa$, effectively increases with increasing strain, see Fig. 7. Individually, Seeback co-efficient increases with increasing strain, while for $G$ and $\kappa$ it is the opposite. Although, the maximum efficiency $\eta(P_{\text{max}})$ and maximum power $P_{\text{max}}$ generated for this system are better than comparable QHE's proposed, the dimension of the considered heat engines, as in the Figs. 2-7, is large $(20 \times 40 nm^2)$. An effective QHE should deliver high power with high efficiency and its dimensions should be as small as possible, so that in less area more number of nano heat engines can be fabricated, and thus total generated power would be large. From Fig. 8(a), we see that with increasing strain(150meV) but decreasing the length ($L = 21nm$) of the strained region, massive power can be generated at high efficiency. The performance of the heat engine can be increased further by tuning one more variable,
the Fermi velocity $v_f$. We have considered the Fermi velocity of Dirac electrons to be equal to $10^6$ m/s, but increasing strain reduces the Fermi velocity to around $6 \times 10^5$ m/s, the performance of the QHE can thus increase further, such that the maximum power as well as efficiency at maximum power both are enhanced to values as high as $0.28 (k_BT)^2/h$ and $0.11 \eta_c$ respectively, see Fig. 8 (b). This can be understood better, if a $1cm^2$ area is occupied by our proposed nanoscale QHE's in parallel, then 0.06 Watts total power can be generated with an efficiency of 0.1 $\eta_c$, which is better than quantum Hall heat engines, see Table 1.

Increasing temperature, Seebeck coefficient and electrical conductance both can be increased to a large value with a maximum power more than $0.2 (k_BT)^2/h$ (at $v_f = 10^6$ m/s) and efficiency at maximum power also more than $0.1\eta_c$. But then the phonon contribution to the thermal conductivity comes into play and that increases the thermal conductivity, implying a reduction in $ZT$, thermodynamic figure of merit. This in turn reduces the efficiency at maximum power, though it does not affect the power of the QHE. We do not consider the phonon contribution, hence in our calculations and Figures plotted have restricted ourselves to an upper limit for temperature of 30K, at which the phonon contribution can be safely neglected.

### Table I. How does the strained graphene QHE compare with related proposals?

| Heat Engines                             | Maximum Power $P_{\text{max}} (k_BT)^2/h$ | Efficiency at maximum Power $\eta(P_{\text{max}})$ | Power generated in $1cm^2$ area fabricated by nano engines |
|------------------------------------------|------------------------------------------|--------------------------------------------------|--------------------------------------------------------|
| Quantum Hall Heat Engine (two terminal)  | 0.14                                    | 0.042 $\eta_c$                                   | 0.04 W                                                  |
| Quantum Hall Heat Engine (three terminal)| 0.14                                    | 0.10 $\eta_c$                                    | 0.04 W                                                  |
| Chaotic Cavity                           | 0.0066                                  | 0.01 $\eta_c$                                    | 0.00189 W                                               |
| Strained Graphene QHE                    | 0.28                                    | 0.1 $\eta_c$                                     | 0.06 W                                                  |

V. CO-EFFICIENT OF PERFORMANCE

Finally we discuss the use of our model as a quantum refrigerator. As in our model external magnetic field is absent, so Time-Reversal symmetry (TR) is not broken. The co-efficient of performance of the refrigerator is defined by the ratio of heat current extracted from the hot reservoir to the electrical power $P$, such as

$$\eta' = \frac{j^q}{P}$$

which is maximum, considering $j^q < 0$ and $P < 0$, for

$$\mathcal{E} = \frac{L^{22}}{L^{21}} (-1 - \sqrt{\frac{L^{11}L^{22} - L^{12}L^{21}}{L^{11}L^{22}}} \Delta T)$$

and, $\eta'_{\text{max}} = \eta_c \sqrt{ZT + 1 - \frac{1}{ZT + 1 + 1}}$

where $\eta_c = \frac{L}{\Delta T}$ is the efficiency of an ideal refrigerator. For the systems with broken TR symmetry, the upper bound of the refrigerator efficiency $\eta'_{\text{max}}$ is always less than $\eta_c$. For systems with conserved TR symmetry, the asymmetric parameter $x = TL^{12}/L^{21}$ becomes unity, and the upper bound of the corresponding maximum efficiency $\eta_{\text{max}}$ equals $\eta_c$. This is the advantage of systems with conserved TR symmetry, that it can work as both heat engine as well as a refrigerator, but for systems with broken TR symmetry, they can only work as a heat engine.

VI. CONCLUSION

We show here that strain acting solely can act as a QHE with better performance characteristics like high efficiency than most other QHE like quantumHall heat engine, chaotic cavity QHE, etc. It has some advantage over magnetically driven QHE. Application of magnetic field breaks the TR symmetry, which in turn reduces the performance of the system as a refrigerator. On the other hand, strain does not break TR symmetry, so our system can act as both heat engine as well as refrigerator. In Table 1 we compare efficiency $\eta(P_{\text{max}})$, power $P_{\text{max}}$, and total power generated for some configured quantum heat engines. We see that our model system has excellent characteristics compared to other QHE’s. This raises a question that perhaps large power and efficiency can also be found with different kind of strain patterns in multi-terminal graphene system, for which further investigations are needed.

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