Curvature-Induced Electrical Properties of Two-Dimensional Electrons on Carbon Nanotube Springs

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SUPPLEMENTARY NOTE 1: PARAMETER JUSTIFICATION

In our numerical calculations, we utilized the parameters r_0,ω_0, and ρ_0 derived from the experimental data analysis in Kim's work [1]. These parameters were essential for establishing the curvature properties and strain-induced effects in our model. The selection of these parameters was guided by experimental results, ensuring consistency between theoretical predictions and observed data.Moreover,r_0, ω_0 and ρ_0 represent the helical radius of the CNT spring, the width of the helical pitch, and the radius of the nanotube, respectively.

These values were extracted from the reported CNT spring properties in Kim's experimental studies [1]. The experimental setup in Kim's work involved controlled mechanical strain application, where current generation was observed under varying strain conditions. Furthermore, in addition to ω_0 and ρ_0 from Kim's work, we incorporated the parameter $\alpha$from Feng's study [2].The parameter α represents the rising angle of the nanospring, describing the inclination of the helical structure relative to its axis. Using α, we determined r_0 more accurately by applying the geometrical relationship:

$$\tan(\alpha) = \frac{\omega_0}{2\pi r_0} \tag{S1}$$

Furthermore, we have presented a table summarizing the relationships between the parameters used in our study through Equation (S1). This table provides a clear depiction of how these parameters interact and contribute to our theoretical framework.

Table S1. Summary of Parameter Relationships in the Theoretical Framework

Parameters	No strain applied	applied 30% strain(compression)
ω_0	90 μm	75 μm
α	34°	50°
r_0	21.23 μm	10.01 μm
ρ_0	10 nm	10 nm

For our theoretical calculations and modeling, we used the parameters obtained under the no-stress applied condition. These values provide the baseline characteristics of the CNT spring before any external strain is introduced.The values of $\omega_0 = 90\mu$m , $r_0 = 21.23\mu m$ and$\rho_0 = 10nm$ were used as the initial parameters in our model. These parameters define the natural curvature and geometry of the CNT spring and were fundamental in establishing the strain-free state. By using these baseline values, we ensured that our theoretical predictions aligned with experimental observations before applying external strain.

SUPPLEMENTARY NOTE 2: HAMILTONIAN FORMULATION

The application of mechanical strain leads to variations in the helical pitch width ω_0 of the CNT spring, which in turn affects the curvature parameter and the Lam'e coefficient $h(s,\phi,t)$. This supplement presents a comprehensive derivation and analysis of Equation (26) in the main paper, incorporating these effects and explaining the approximations used in obtaining the final expression. Under applied strain, the helical pitch width varies with time as:

$$\omega(t) = \omega_0 + \Delta\omega \sin(\Omega t) \tag{S2}$$

Due to the variation of ω_0 under applied strain, the curvature parameter ($\kappa_0 = \frac{1}{r_0(1+\frac{\omega_0}{r_0})^2}$) varies with time:

$$\kappa(t) = \frac{1}{r_0(1+(\frac{\omega_0(t)}{r_0})^2)} \tag{S3}$$

Replacing $\omega(t)$ in the curvature parameter expression, we obtain:

$$\kappa(t) = \frac{1}{r_0\left(1+\frac{\omega_0^2}{r_0^2}\right)\left(1+\frac{2\omega_0\Delta\omega\cos(\Omega t)+\Delta\omega^2\cos^2(\Omega t)}{\left(1+\frac{\omega_0^2}{r_0^2}\right)r_0^2}\right)}$$

Next, we approximate the curvature parameter using the first-order Taylor expansion $\frac{1}{(1+x)} \approx 1-x$. The curvature parameter can be divided into a time-independent term κ_0 and a time-dependent term $\Delta\kappa(t)$:

$$\kappa(t) = \kappa_0 + \Delta\kappa(t) \tag{S4}$$

$$\Delta\kappa(t) = \left(\frac{1}{a_0^4 r_0^3}\right)\left(\Delta\omega^2\sin^2(\Omega t) - 2\omega_0\Delta\omega\sin(\Omega t)\right) \tag{S5}$$

Next, we consider the Hamiltonian of the system, as presented in Eq. 15 in the main paper:

$$\hat{\mathbf{H}} = \frac{1}{\rho_0}\gamma^0\gamma^1\partial_\phi + \frac{1}{h(s,\phi)}\gamma^0\gamma^2\partial_s + \frac{1}{2\rho_0}\gamma^0\gamma^1\partial_\phi \ln h(s,\phi) \tag{S6}$$

The influence of strain on the curvature parameter causes the Lam'e coefficient to vary with time. Considering $\frac{1}{h(s,\phi,t)}$ in the Hamiltonian, we express it as:

$$\frac{1}{h(s,\phi,t)} = \frac{1}{(1+\kappa_0\rho_0\cos(\theta(s)+\phi))} \cdot \frac{1}{\left(1+\frac{\Delta\kappa(t)\rho_0\cos(\theta(s)+\phi)}{1+\kappa_0\rho_0\cos(\theta(s)+\phi)}\right)} \tag{S7}$$

Using the first-order Taylor expansion approximation $\frac{1}{(1+x)} \approx 1-x$:

$$\frac{1}{\left(1+\frac{\Delta\kappa(t)\rho_0\cos(\theta(s)+\phi)}{1+\kappa_0\rho_0\cos(\theta(s)+\phi)}\right)} = 1 - \frac{\Delta\kappa(t)\rho_0\cos(\theta(s)+\phi)}{1+\kappa_0\rho_0\cos(\theta(s)+\phi)} \tag{S8}$$

Thus,

$$\frac{1}{h(s,\phi,t)} = \frac{1}{h_0 + \frac{\Delta h(t)}{h_0^2}} \tag{S9}$$

where $\Delta h(t) = \Delta\kappa(t)\rho_0\cos(\theta(s)+\phi)$. Next, we consider the term $\partial_\phi \ln h(s,\phi,t)$ by substituting $h(s,\phi,t) = \frac{h_0^2}{h_0+\Delta h(t)}$, which gives:

$$\partial_\phi \ln h(s,\phi,t) = 2\partial_\phi \ln h_0 + \partial_\phi \ln(h_0 + \Delta h(t)) \tag{S10}$$

By incorporating Eq. (S9) and Eq. (S10) into the Hamiltonian, it can be divided into an unperturbed term $\hat{\mathbf{H}}0(\kappa 0)$ and a perturbed term $\hat{\mathbf{H}}_I(\kappa(t))$:

$$\hat{\mathbf{H}}(\kappa(t)) = \hat{\mathbf{H}}0(\kappa 0) + \hat{\mathbf{H}}_I(\kappa(t)) \tag{S11}$$

Here, $\hat{\mathbf{H}}0(\kappa 0)$ represents the unperturbed Hamiltonian of the CNT spring system without external strain, and $\hat{\mathbf{H}}_I(\kappa(t))$ is the perturbation term induced by applied strain. This perturbation term accounts for changes in the helical pitch width, affecting the Lam'e coefficient and curvature parameters over time. The perturbation term is given by:

$$\hat{\mathbf{H}}_I(\kappa(t)) = \frac{\Delta h(t)}{h^2 0}\gamma^0\gamma^2\partial_s - \frac{1}{2}\gamma^0\gamma^1\rho_0\partial_\phi \ln(h_0 + \Delta h(t)) \tag{S12}$$

REFERENCES

1. Kim,S.H.;et al.Harvesting electrical energy from carbon nanotube yarn twist. *Science* **2017**, *357*,773-778.
2. Feng, C.; Liew, K. M.Structural stability of carbon nanosprings. *Carbon* **2011**, *49*,4688-4694.