Steady states of driven matter

I will present a striking theoretical example of possibility of controlling the properties of materials by driving them out of equilibrium.

Iadecola et al. PRL (2013), PRB (2013)

1) Describe a mechanism for opening a tunable Kekule gap in graphene by exciting an optical phonon mode at the Dirac point K_+ or K_-. This gap corresponds to a complex-valued order parameter Δ that rotates in time.

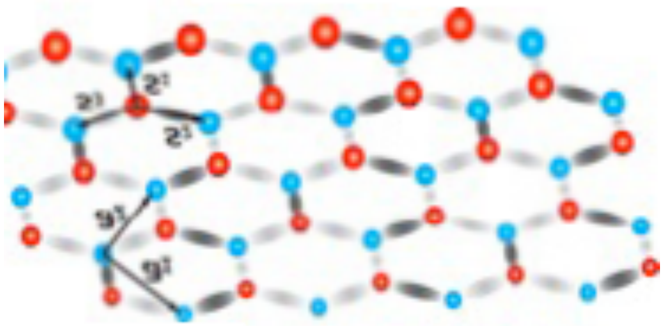
2) Show that the system reaches a steady state whose transport properties are the same as if the system had a static electronic gap, controllable by the driving amplitude.

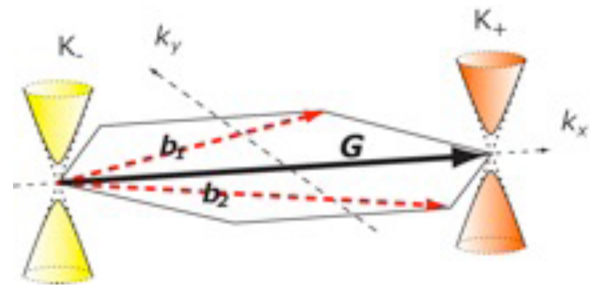
3) Analyze our driven graphene through the lens of Floquet theory

Our exactly soluble driven graphene system plays the role of hydrogen atom / H.O. in the study of driven matter. It provides understanding of the notion of quasi-energy in Floquet theory.

Static Kekule Distortion:

Static Kekule distortion is a particular dimerization of lattices, which corresponds to coupling points in the BZ that are separated by the two Dirac points.





$$G = K_+ - K_-$$

If it occurs, it opens a gap in graphene. In addition, fractionally charged statescan emerge that are bound to vortices in the order parameter $\Delta\,(\boldsymbol{r})$. Charge fractionalization in graphene has been studied extensively due to the fact that it is the first realization of 2 – D fractional charge.

However, Kekule distortion has not been seen.

Dynamic Kekule distortion: Generation of rotating mass

We consider the **time–dependent** Kekule distortion that results from the excitation of the highest–energy optical phonon modes at wave vectors $\boldsymbol{K}_{\pm}$ with frequency Ω (Kekule phonon).

Suzuura and Ando, J. Phys. Soc. Jpn. (2008)

We find the time–dependent order parameter has the form,

$$\Delta\,(\tau) = |\Delta|\, e^{i\,(\Omega\, t\, + \varphi)}$$

when K_{+} point is excited. $|\Delta|$ depends on the amplitude of the excited waves, and therefore the magnitude of order parameter is controllable.

[K_{-} mode is obtained by $\Omega \to -\Omega$.]

The resulting **time dependent** tight-binding Hamiltonian is

$$H = -\sum_{r\in\Lambda_A} \sum_{j=1}^{3} \left[t + \delta t_{r,j}\,(\tau)\right] a_r^\dagger\, b_{r+s_j} + \text{H.c.}$$

[Note: *H* includes spatial fluctuations.]

The corresponding Lagrangian in the continuum may be written as

$$\mathcal{L} = \overline{\Psi}\,\left[\gamma^\mu \left(i\,\partial_\mu + \gamma^5 A_{5\mu}\right) - |\Delta|\, e^{-i\gamma^5(\Omega\,\tau + \varphi)}\right]\Psi$$

The spatial part of the axial gauge fields, A_{5i} , corresponds to acoustic phonons and strain in the lattice.

Axial gauge fields play an important role in the asymptotic steady state of the driven system providing a thermal bath for our system.

Dirac Hamiltonian for the system subject to the **time-dependent** Kekule texture is

$$\mathcal{H}_{sys}(\tau) = \begin{pmatrix} \boldsymbol{\sigma} \cdot \boldsymbol{p} & \Delta\, e^{i\Omega\tau} 1 \\ \Delta^* e^{-i\Omega\tau}\, 1 & -\boldsymbol{\sigma} \cdot \boldsymbol{p} \end{pmatrix}$$

How to understand the state of a system that is both strongly driven and coupled to a thermal bath?

$$\mathcal{L} = \bar{\Psi}\left[\gamma^\mu\left(i\,\partial_\mu + \gamma^5 A_{5\mu}\right) - |\Delta|\, e^{-i\gamma^5(\Omega\,\tau + \varphi)}\right]\Psi$$

Key observation: The time-dependent mass term in $\mathcal{L}$ can be removed by the following axial (valley) gauge transformation!

Jackiw and Pi, PRL (2007)

$$\Psi' = e^{-i\,\gamma^5\,\Omega\,\tau/2}\,\Psi\,, \qquad A'_{50} = A_{50} + \Omega/2\,, \qquad A'_{5i} = A_{5i}$$

$$\Longrightarrow \qquad \mathcal{L}' = \overline{\Psi'}\left[\,\gamma^\mu\left(i\,\partial_\mu + \gamma^5 A'_{5\mu}\right) - |\Delta|\, e^{-i\gamma^5\varphi}\,\right]\Psi'$$

Lagrangian in **"comoving"** frame ("rotating" frame)

Response functions are invariant under the axial gauge transformation:

Vector current operator $\qquad j^\mu = \bar{\Psi}\,\gamma^\mu\,\Psi$

Axial vector current operator $\qquad j_5^\mu = \bar{\Psi}\,\gamma^\mu\,\gamma_5\,\Psi$

The gauge transformation removes time-dependence completely, including the system – bath coupling $A_{5i}\, j_5^i$!

Non–equilibrium steady state

↓

Thermal equilibrium in the comoving frame

The Hamiltonian for the system in the “comoving “ frame (without the bath)

$$\mathcal{H}'_{sys} = \begin{pmatrix} \boldsymbol{\sigma}\cdot\boldsymbol{p} + \frac{\Omega}{2}\,1 & |\Delta|\,e^{i\varphi}\,1 \\ |\Delta|\,e^{-i\varphi}1 & -\boldsymbol{\sigma}\cdot\boldsymbol{p} - \frac{\Omega}{2}\,1 \end{pmatrix}$$

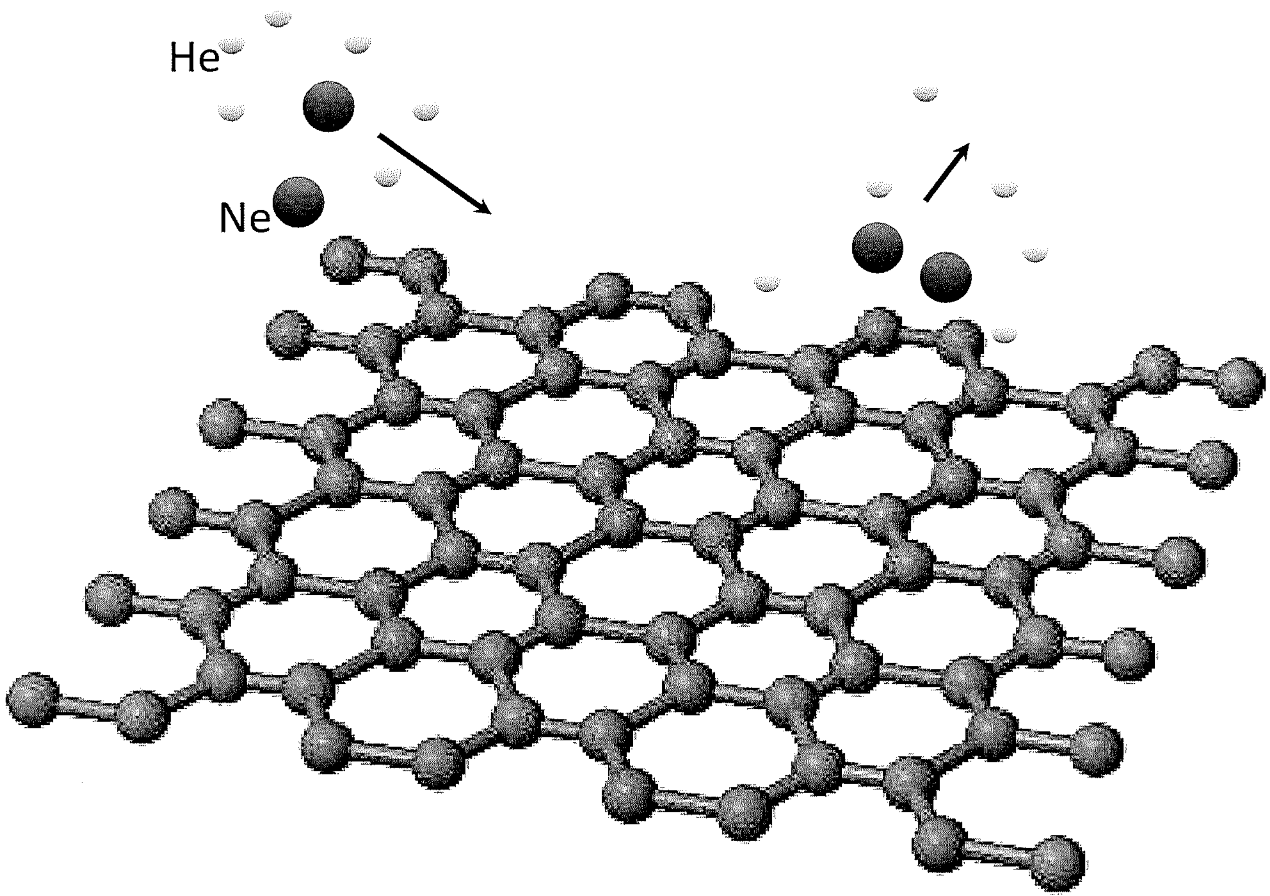
$$E_{\pm,\mp} = \pm\sqrt{(p \mp \frac{\Omega}{2})^2 + |\Delta|^2}$$

All observables associated with the current operator can be computed in the comoving frame.

The driven system behaves as a semiconductor with a gap tunable by the amplitude of the Kekule mode.

Size of the gap is ~0.025 eV for 0.04% displacement of the graphene atoms from equilibrium.

Possible experimental realization



Goldberg and El-Batanouny Groups, Boston University (in progress)

Floquet theory: a popular approach

Analysis of driven graphene through the lens of Floquet theory:

What can we learn about Floquet theory?

Periodically driven quantum system: $H(t) = H(t+T), \; T = \frac{2\pi}{\Omega}$

Floquet's Theorem: $H(t)\left|\Psi_\alpha(t)\right\rangle = i\partial_t \left|\Psi_\alpha(t)\right\rangle$

$$\Longrightarrow \left|\Psi_\alpha(t)\right\rangle = e^{-i\epsilon_\alpha t}\left|\Phi_\alpha(t)\right\rangle$$

1) "**Floquet states**" $\left|\Phi_\alpha(t)\right\rangle$ share periodicity of Hamiltonian:

$$\left|\Phi_\alpha(t)\right\rangle = \left|\Phi_\alpha(t+T)\right\rangle$$

2) "**Quasi-energies**" ϵ_α solve **Floquet eigenvalue problem:**

$$\left[H(t) - i\partial_t\right]\left|\Phi_\alpha(t)\right\rangle = \epsilon_\alpha \left|\Phi_\alpha(t)\right\rangle$$

Quasi-energy spectrum is only defined mod Ω!

$$|\Psi_\alpha(t)\rangle = e^{-i\epsilon_\alpha t}\,|\Phi_\alpha(t)\rangle$$

Shifting $\epsilon_\alpha \to \epsilon_\alpha + m\Omega$ leaves definition unchanged

↓

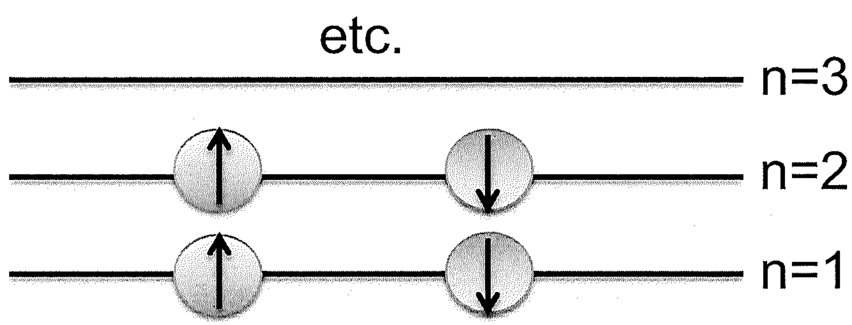
Floquet states with quasi-energies ϵ_α and $\epsilon_\alpha + m\Omega$
are not physically distinct!

What does this mean?

Un-driven systems have a principle:

Higher energies are penalized (less probable)

Fermions at T=0: Fill states in the order that minimizes E



T≠0: Higher-energy states are penalized exponentially

$$P(E) \propto e^{-\beta E}$$

Quasi-energies need not obey this principle!

Relation to Floquet theory

We want to solve the Floquet eigenvalue problem:

$$[H(t) - i\partial_t] \, |\Phi_\alpha(t)\rangle = \epsilon_\alpha \, |\Phi_\alpha(t)\rangle$$

Easiest to work in frequency domain:

$$|\Phi_\alpha(t)\rangle = |\Phi_\alpha(t+T)\rangle \implies |\Phi_\alpha(t)\rangle = \sum_{n=-\infty}^{\infty} e^{-in\Omega t} \, |\Phi_\alpha^n\rangle$$

$$\sum_{n=-\infty}^{\infty} (\mathcal{H}_{mn} - n\Omega \, \delta_{mn}) \, |\Phi_\alpha^n\rangle = \epsilon_\alpha \, |\Phi_\alpha^m\rangle$$

$$\mathcal{H}_{mn} = \frac{1}{T} \int_0^T dt \; e^{i(m-n)\Omega t} \; \mathcal{H}_{\text{sys}}(t)$$

Infinite-dimensional eigenvalue problem!

$$\mathcal{H}_{\text{sys}}(t) = \begin{pmatrix} \boldsymbol{\sigma} \cdot \boldsymbol{p} & \Delta \, e^{i\Omega t} \, \mathbb{1} \\ \Delta^* \, e^{-i\Omega t} \, \mathbb{1} & -\boldsymbol{\sigma} \cdot \boldsymbol{p} \end{pmatrix}$$

Exact Floquet solution

For our model, $\mathcal{H}_{mm} \equiv \mathcal{H}_0 = \begin{pmatrix} \boldsymbol{\sigma}\cdot\boldsymbol{p} & 0 \\ 0 & -\boldsymbol{\sigma}\cdot\boldsymbol{p} \end{pmatrix}$ $\mathcal{H}_{m\,m+1} \equiv \mathcal{H}_1 = \begin{pmatrix} 0 & \Delta\,\mathbb{1} \\ 0 & 0 \end{pmatrix}$

$$\mathcal{H}_{m\,m-1} \equiv \mathcal{H}_{-1} = \begin{pmatrix} 0 & 0 \\ \Delta^*\,\mathbb{1} & 0 \end{pmatrix} \qquad \mathcal{H}_{mn} = 0 \qquad \text{if } |m-n| > 1.$$

Can write Floquet equation in matrix form:

$$\begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \\ \cdots & \mathcal{H}_0 - \Omega\,\mathbb{1} & \mathcal{H}_1 & 0 & \cdots \\ \cdots & \mathcal{H}_{-1} & \mathcal{H}_0 & \mathcal{H}_1 & \cdots \\ \cdots & 0 & \mathcal{H}_{-1} & \mathcal{H}_0 + \Omega\,\mathbb{1} & \cdots \\ & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ |\Phi_\alpha^1\rangle \\ |\Phi_\alpha^0\rangle \\ |\Phi_\alpha^{-1}\rangle \\ \vdots \end{pmatrix} = \epsilon_\alpha \begin{pmatrix} \vdots \\ |\Phi_\alpha^1\rangle \\ |\Phi_\alpha^0\rangle \\ |\Phi_\alpha^{-1}\rangle \\ \vdots \end{pmatrix}$$

Now just truncate matrix and diagonalize:

~~$\epsilon^0_{\pm,\pm} = \pm p \pm m_0 \Omega$~~ ← Depends on truncation size!

$$\epsilon^n_{\pm,\pm,\pm} = \pm\sqrt{(p \pm \Omega/2)^2 + |\Delta|^2} \pm \frac{n\Omega}{2}$$

← Holds for all n=0,…,∞

- The spectrum of system's Floquet effective Hamiltonian $\mathcal{H}_{\text{eff}}$ is obtained by choosing a single quasi-energy branch, say n=1, without loss of generality.

  $\Longrightarrow$

  The quasi-energies $\epsilon^{1}_{\pm,\pm,+}$ are identical to the energy eigenvalues $E_{\pm,\pm}$ of our time-independent $\mathcal{H}'$ in the rotating frame, up to a constant shift by $-\Omega/2$.

  This indicates that the rotating-frame Hamiltonian $\mathcal{H}'$ can be identified with $\mathcal{H}_{\text{eff}}$ of Floquet Theory.

- The time-dependent Hamiltonian $\mathcal{H}_{\text{sys}}(t)$ is related to $\mathcal{H}'$ $(= \mathcal{H}_{\text{eff}})$ by a unitary transformation

$$\mathcal{H}' = U(t)\, \mathcal{H}_{\text{sys}}(t)\, U^{\dagger}(t) - i\, U(t)\, \partial_t\, U^{\dagger}(t)$$

$$U(t) = e^{-i\,\gamma^5\,\Omega\, t/2}$$

Summary

1) Driven systems may host many novel phenomena, but pose challenges to theoretical understanding.

2) We studied possibility of generating Kekule mass in driven graphene.

   a) Can open a tunable gap in graphene by exciting TO phonon mode at either K – point
   b) Transport properties of the system can be understood by transforming to a comoving frame

3) Analyzed our driven graphene through the lens of Floquet theory.

   a) Obtained exact solutions to eigenvalue problem of Floquet Hamiltonian for driven graphene
   b) Our exactly soluble driven graphene system plays the role of hydrogen atom / H.O. in the study of driven matter

      i) Its energies provide understanding of Floquet quasi-energies
      ii) Our Hamiltonian in the rotating system is in fact Floquet Effective Hamiltonian