Kerner's path approach to materials growth and some unexpected connections

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Verazao Cuántico 2023, Brasil

- Introduction

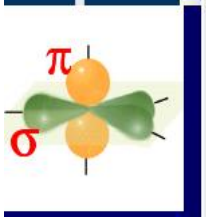
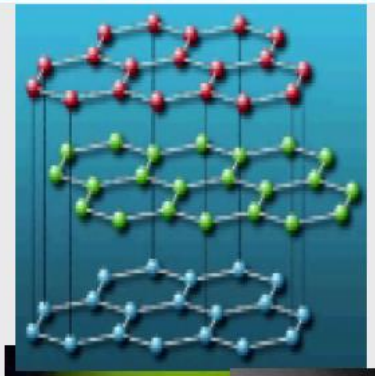
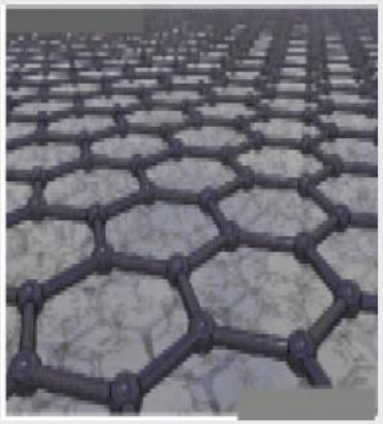
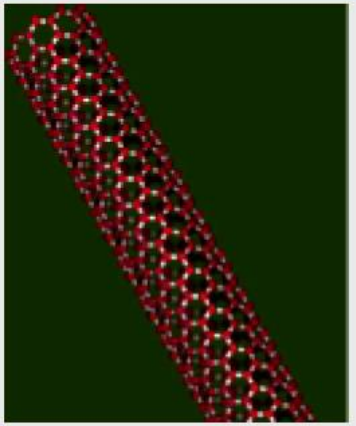
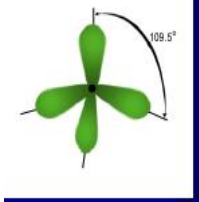
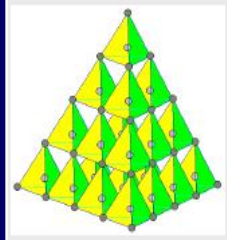
  Richard Kerner's path approach

- 2D Materials: Relativistic quantum equations in curved space

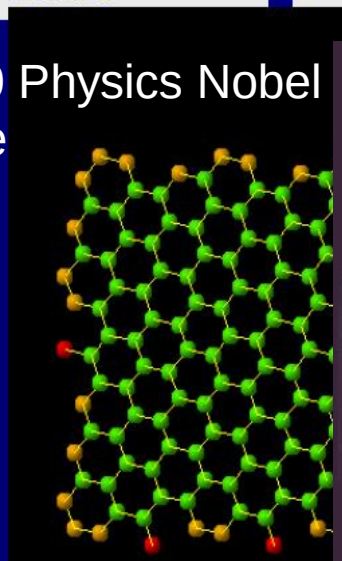
- Superconductivity in Graphene and supersymmetry….

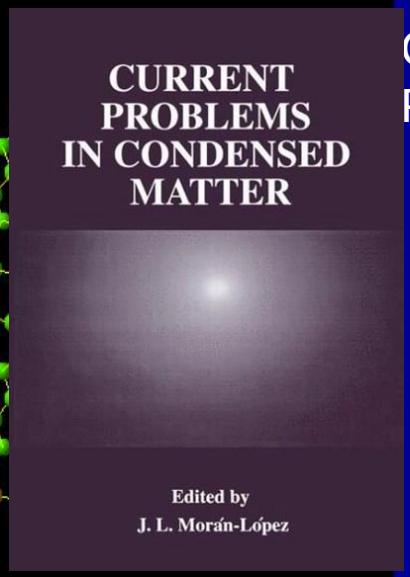
- Conclusions

Carbon allotropes

	3D	2D	1D	0D
sp^2	   graphite	 Graphene 2005	 Carbon nanotube Multi-wall1991 Single wall 1993	  Buckyball 1985
sp^3	   diamond			

2010 Physics Nobel Prize



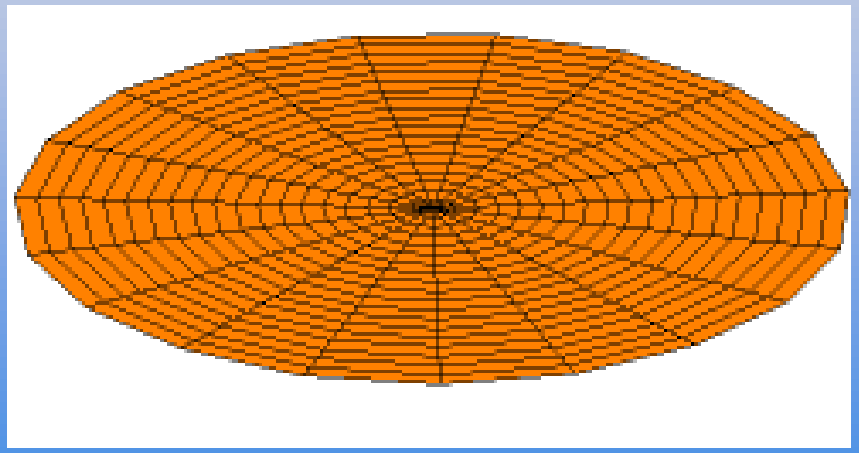


Chemistry Nobel Prize 2011

2010 Physics Nobel Prize

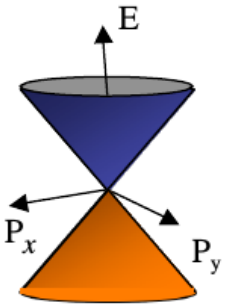
- First “two” dimensional material

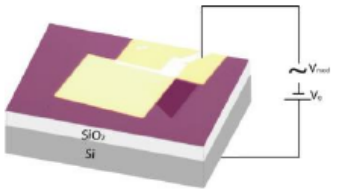
tought to be impossible to exist...



Why the interest ?

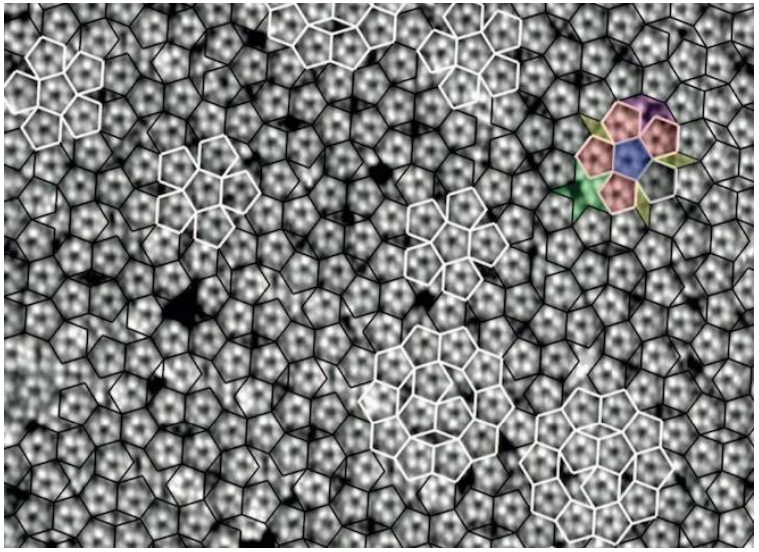
- **2D crystal with extraordinarily few defects**
- **Exotic electrical behaviors**
  - $E = v_F \bullet P$ (massless Dirac fermions)
  - Efficient tunneling through energy barrier, anomalous quantum Hall effects, …
- **Excellent materials properties**
  - Electrical -- high electron mobility, high current carrying capacity,…
  - Mechanical -- large Young's modulus, high tensile strength, low friction, …
  - Thermal -- high thermal conductivity
- **Excellent controllability**
  - Electrical gating, structural patterning, etc





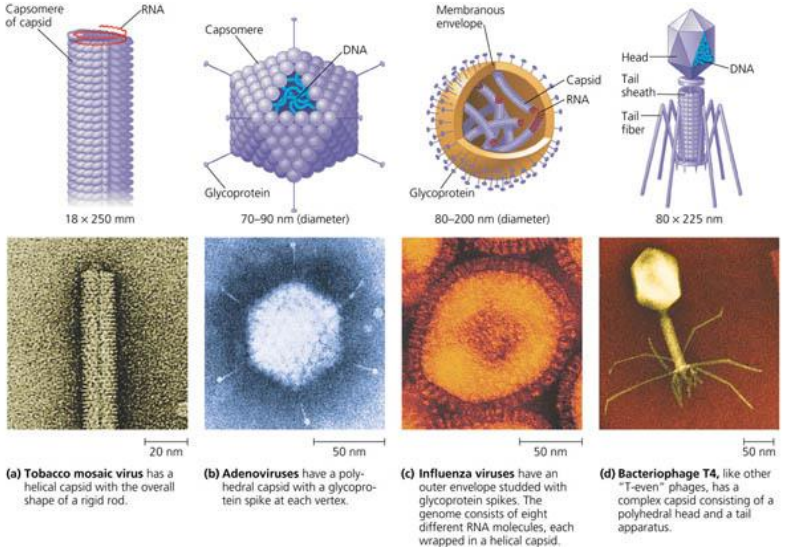
Attractive for fundamental physics and technological applications

Quasicrystals (1984)

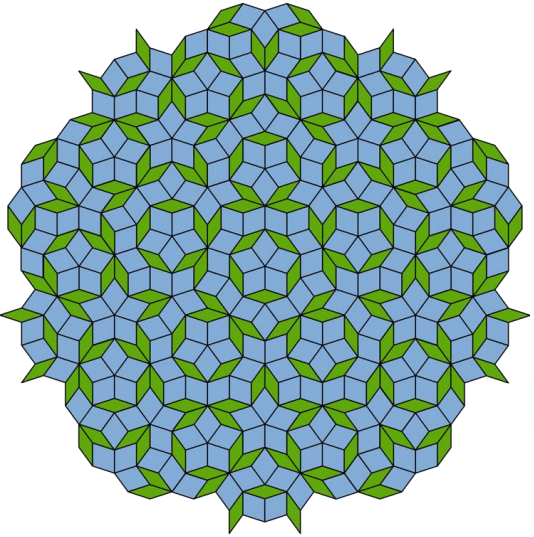


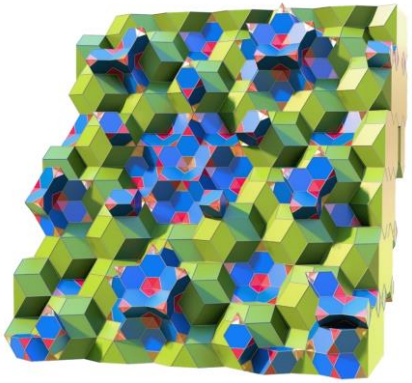
2011 Chemistry Nobel Prize

Virus

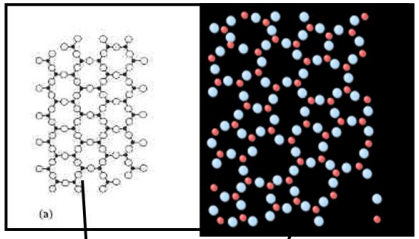


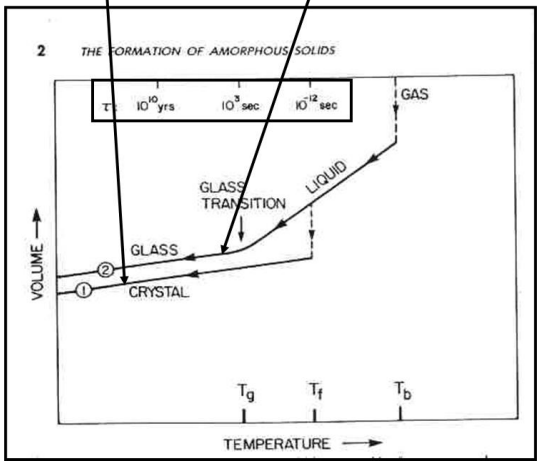
Roger Penrose Tiling (1970's)





Glass Formation





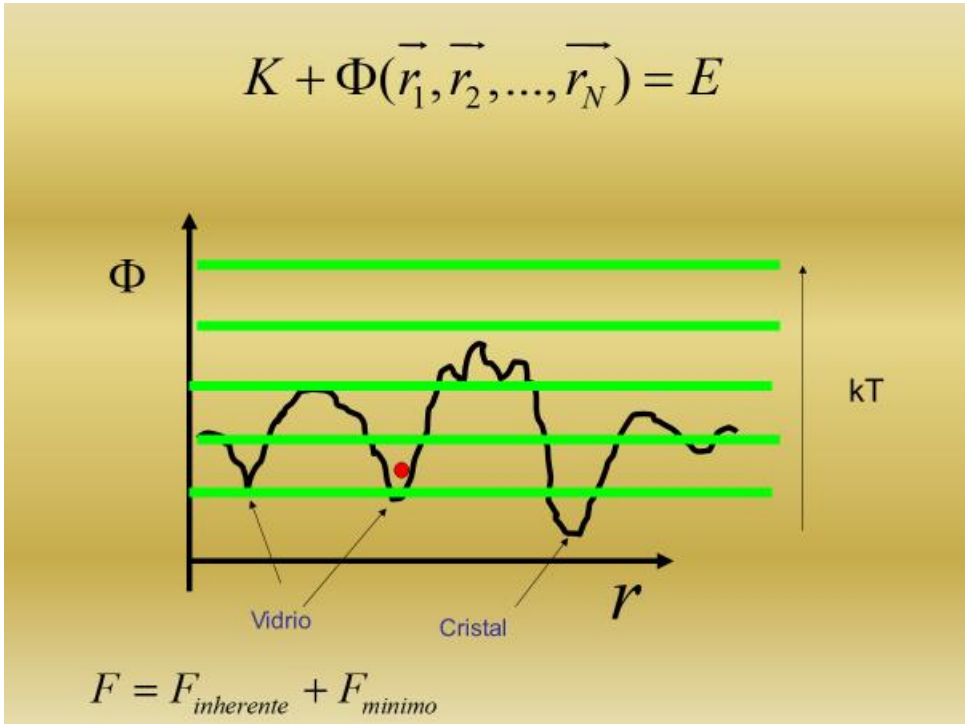
2009 Physics Nobel Prize: optical fibers make possible internet

How such nice structures are assembled?

Usual approach:

1) Hamiltonian $$H = \sum_{i=1}^{N} \frac{P_i^2}{2m} + \Phi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = K + \Phi = E$$

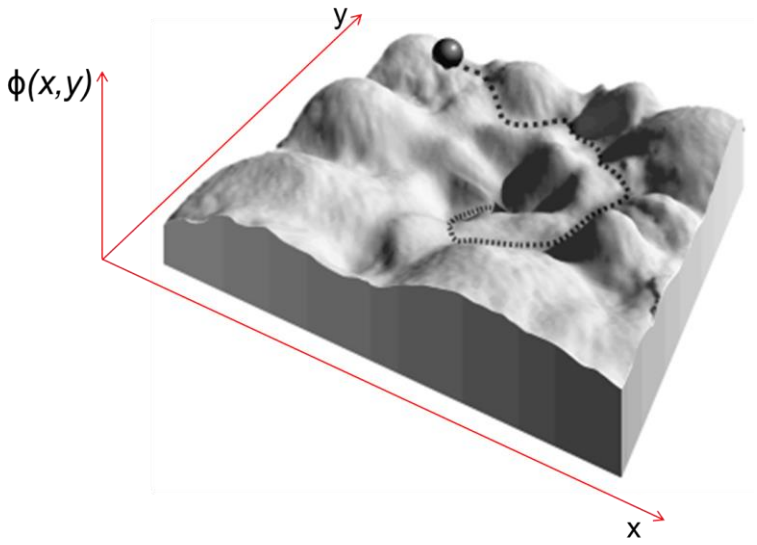
2) Statistical mechanics counting "states" $\longrightarrow (\vec{p}_1, \vec{p}_2, \ldots, \vec{p}_N, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$



$$S = k \ln \Omega(vib.) + k \ln(\#\min(E))$$

All states probed….

Many problems



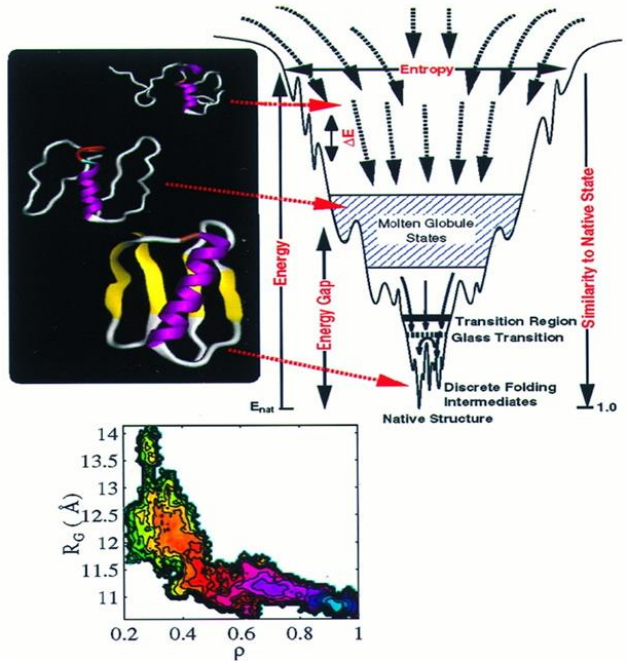
1) “A random search among all possible configurations can take an enormously long time. Yet assembling takes place in seconds or less.”

2) Numerically very challenging

3) Not always an equilibrium process.

4) Without computers, limited prediction power.

Protein Folding



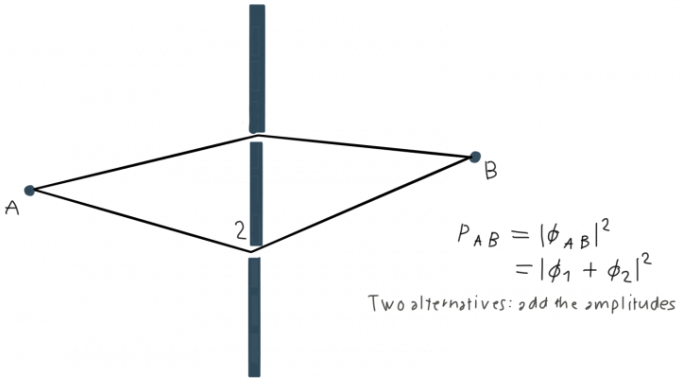
Levinthal (1969): if a protein were to attain its correctly folded configuration by sequentially sampling all the possible conformations, it would require a time longer than the age of the universe to arrive at its correct native conformation.

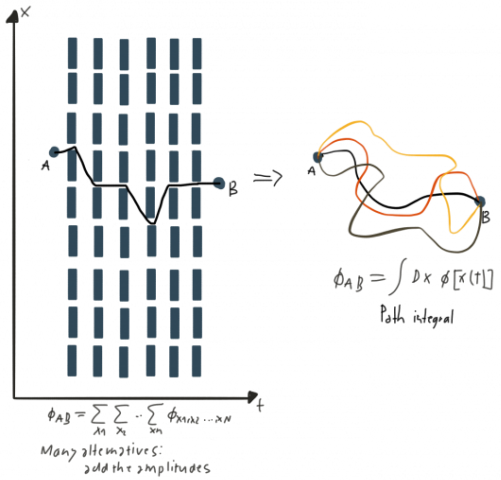
Google's DeepMind AI Predicts 3D Structure of Nearly Every Protein Known to Science
At last, the decades-old protein folding problem may finally be put to rest. (2023)

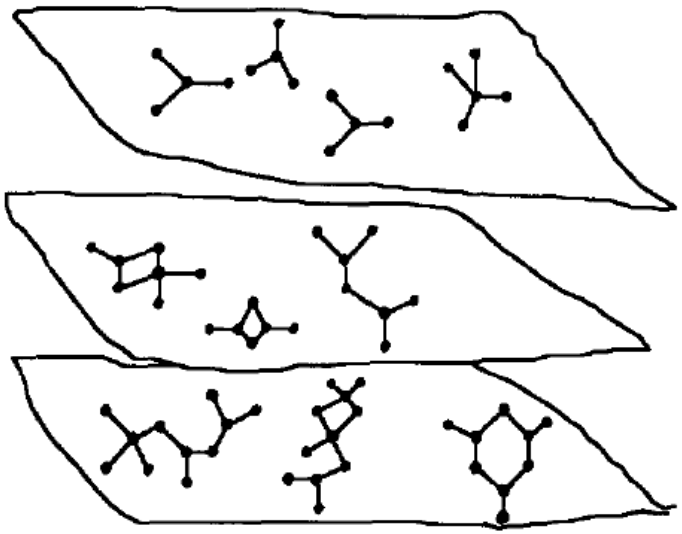
Richard's approach

- Replace space of states by space of all agglomeration paths
  (all posible paths that lead to a certain cluster size)

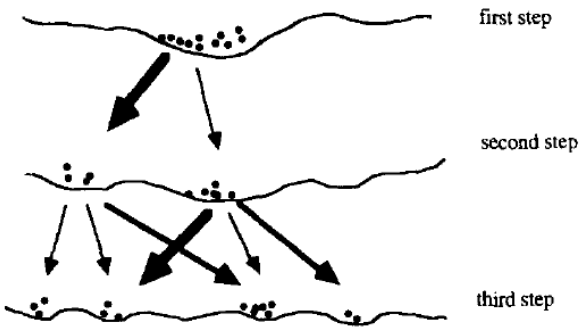
Feynman path approach to QM…







Energy+Entropy



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Computational Materials Science 2 (1994) 500–508

COMPUTATIONAL MATERIALS SCIENCE

Nucleation and growth of fullerenes

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several authors [3–5]. What is rather lacking is a model that besides displaying only purely qualitative features, would also make use of quantities that might be evaluated and measured, such as the bond-bending energies involved, or the activation energies needed to break a single or double bond in the structure. Moreover, a theoretical model, in order to deserve its name, should lead to numerical predictions, e.g. to explain the upper limit of the efficiency of production of C_{60} in the arc (close to 10 % of the collected soot), the relative abundance of other forms of fullerenes, such as C_{70} (less than 1%), and other measurable characteristics of the agglomeration process and the resulting clusters. In order to represent

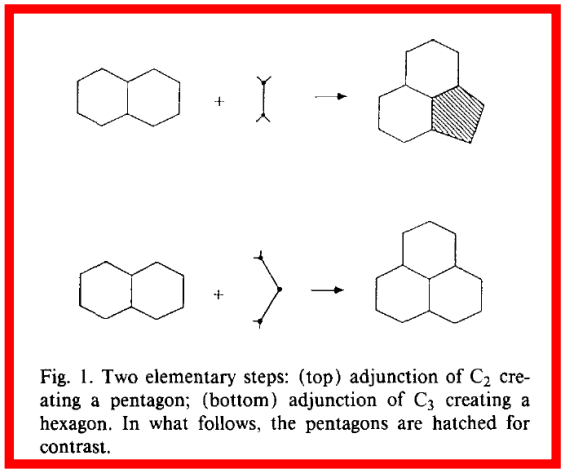
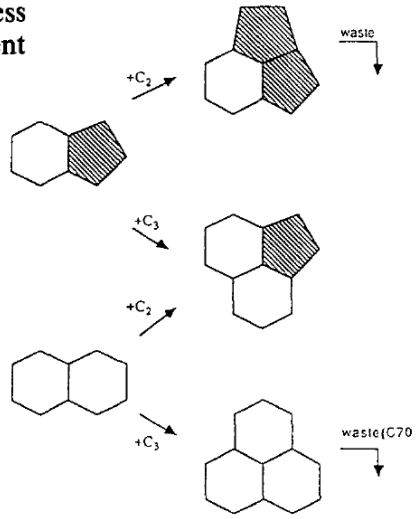
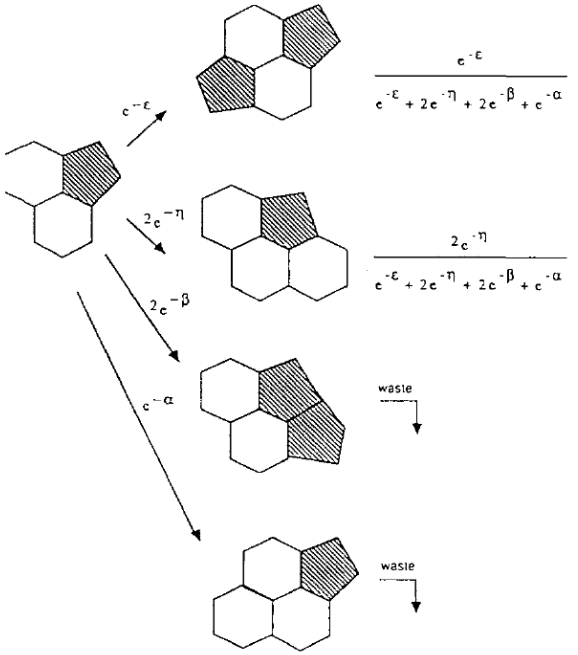


Fig. 1. Two elementary steps: (top) adjunction of C_2 creating a pentagon; (bottom) adjunction of C_3 creating a hexagon. In what follows, the pentagons are hatched for contrast.





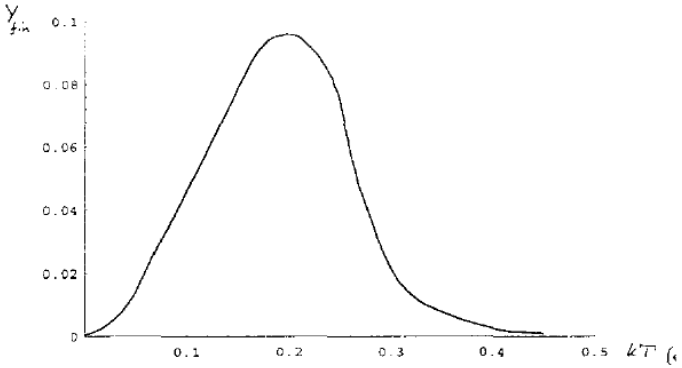
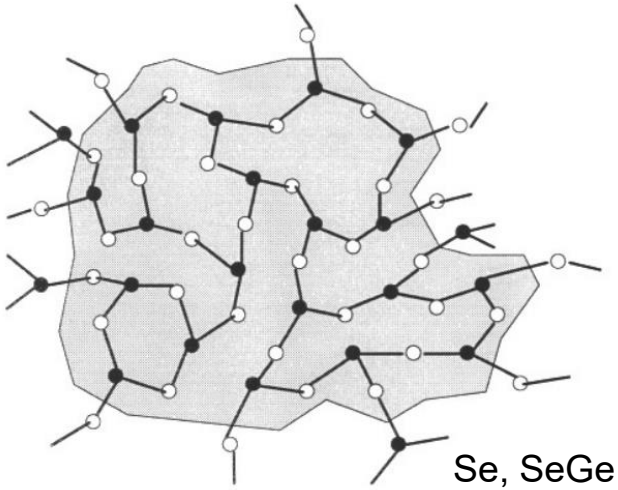
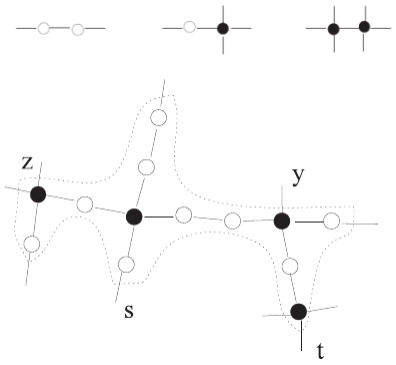


Fig. 6. The yield of C_{60} versus the temperature.

Stochastic Matrix Method: network glasses





$$\mathbf{e}_1 = \frac{1}{4B+7A}(4B, A, 2A, 4A)$$

where A is

$$A = \frac{2c_B\xi}{c_A + 2c_B\xi}$$

and

$$B = \frac{c_A}{c_A\xi + 2c_B\mu}.$$

Se, SeGe , SeAs, SeAsGe,…

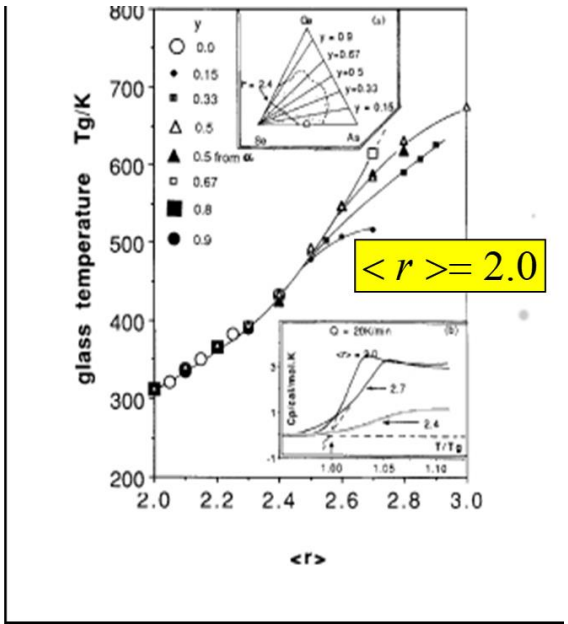
$$M = \begin{pmatrix} 2c_A e^{-E_1/kT} & 2c_A e^{-E_2/kT} & 2c_A e^{-E_2/kT} & 2c_A e^{-E_2/kT} \\ 0 & 0 & 2c_A e^{-E_2/kT} + 4c_B e^{-E_3/kT} & 0 \\ 0 & 0 & 0 & 2c_A e^{-E_2/kT} + 4c_B e^{-E_3/kT} \\ 4c_B e^{-E_2/kT} & 4c_B e^{-E_3/kT} & 4c_B e^{-E_3/kT} & 4c_B e^{-E_3/kT} \end{pmatrix}$$

$$M = \begin{pmatrix} \frac{c_A}{(c_A\xi+2c_B\mu)} & \frac{c_A\xi}{(c_A\xi+2c_B\mu)} & \frac{c_A\xi}{2(c_A\xi+2c_B\mu)} & \frac{c_A\xi}{2(c_A\xi+2c_B\mu)} \\ 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 1/2 \\ \frac{2c_B\xi}{(c_A\xi+2c_B\mu)} & \frac{2c_B\mu}{(c_A\xi+2c_B\mu)} & \frac{2c_B\mu}{2(c_A\xi+2c_B\mu)} & \frac{2c_B\mu}{2(c_A\xi+2c_B\mu)} \end{pmatrix}$$

Recover empirical Gibbs-Di Marzio law!

$$T_g = \frac{T_{og}}{1 - \frac{1}{2\ \ln\ 2}(\langle r\rangle - 2)}$$

First encounter with topology and glasses



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Journal of Non-Crystalline Solids 231 (1998) 111–119

JOURNAL OF NON-CRYSTALLINE SOLIDS

Stochastic matrix description of glass transition in ternary chalcogenide systems

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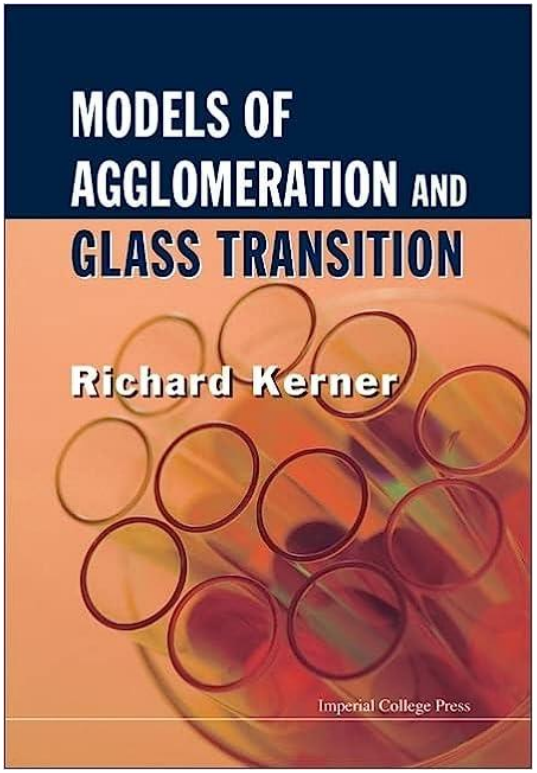
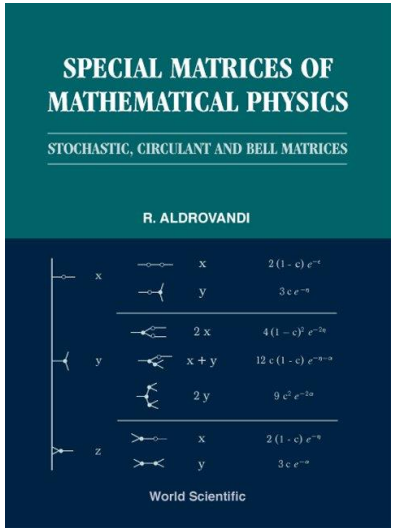
[b] Instituto de Física, Universidad Nacional Autónoma de México, Apdo. Postal 20-364, 01000 México D.F., Mexico

Received 22 December 1997

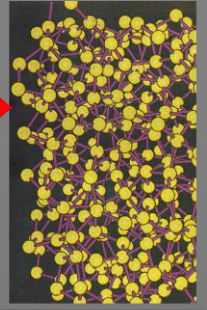


Stochastic Matrices:
Evolving Systems
Markov Chains
Glass Transition
The Kerner Model
Formal Developments
Equilibrium,
Dissipation and
Ergodicity



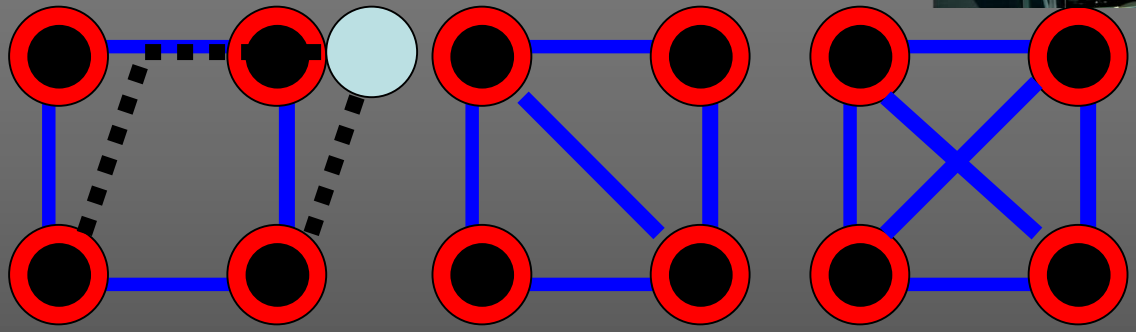
-Quasicrystals
-Glasses
-Virus
-Nanomaterials

Rigidity and topology



Richard introduced me to Jim Phillips in Cambridge meeting

With N hinges, how many bars to make it rigid?



Flexible *Isostatic* *Rigid*

1 *0* *-1*

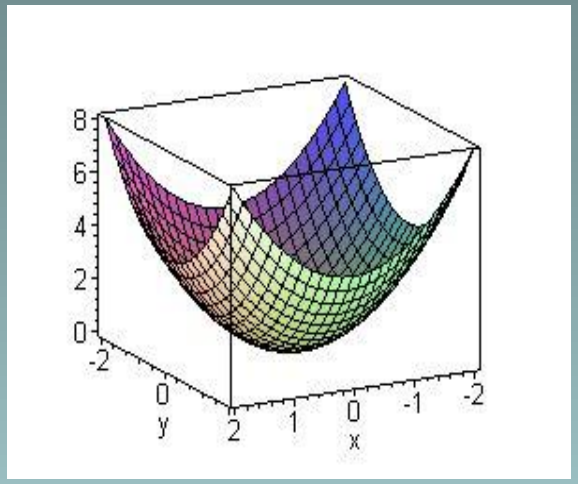
4x (2 freedom degrees)-(# constraints)=# of flexible modes

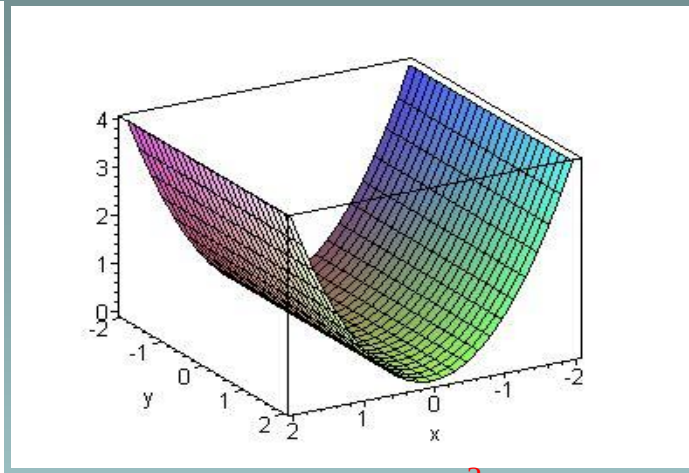
f =(# flexible modes)/3N *Fraction of "floppy", flexible modes*

$$V(x) = \frac{m\omega^2}{2} x^2$$

Topology and Floppy Modes

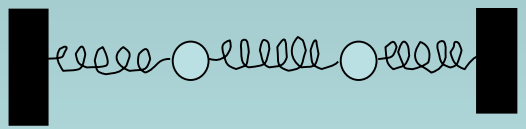
$$V(x,y)=\frac{\alpha_2}{2}(x^2+y^2+(x-y)^2)+\frac{\alpha_3}{3}(x^3+y^3+(x-y)^3)$$



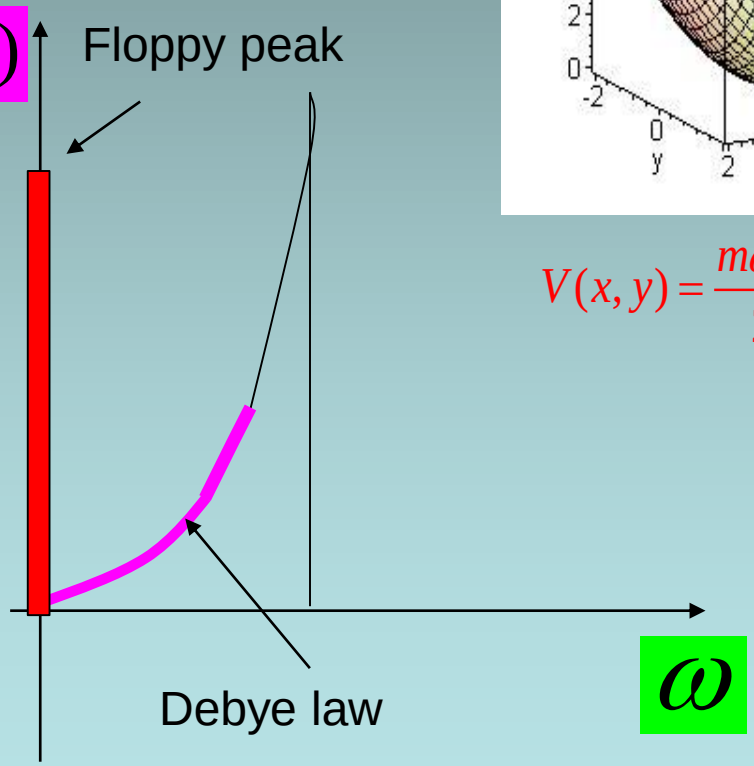


$$V(x,y)=\frac{m\omega^2_1}{2}x^2+\frac{m\omega^2_2}{2}y^2$$

$$V(x,y)=\frac{m\omega^2_1}{2}x^2$$



$$S\approx f\,3Nk_B\ln(V/V_0)$$

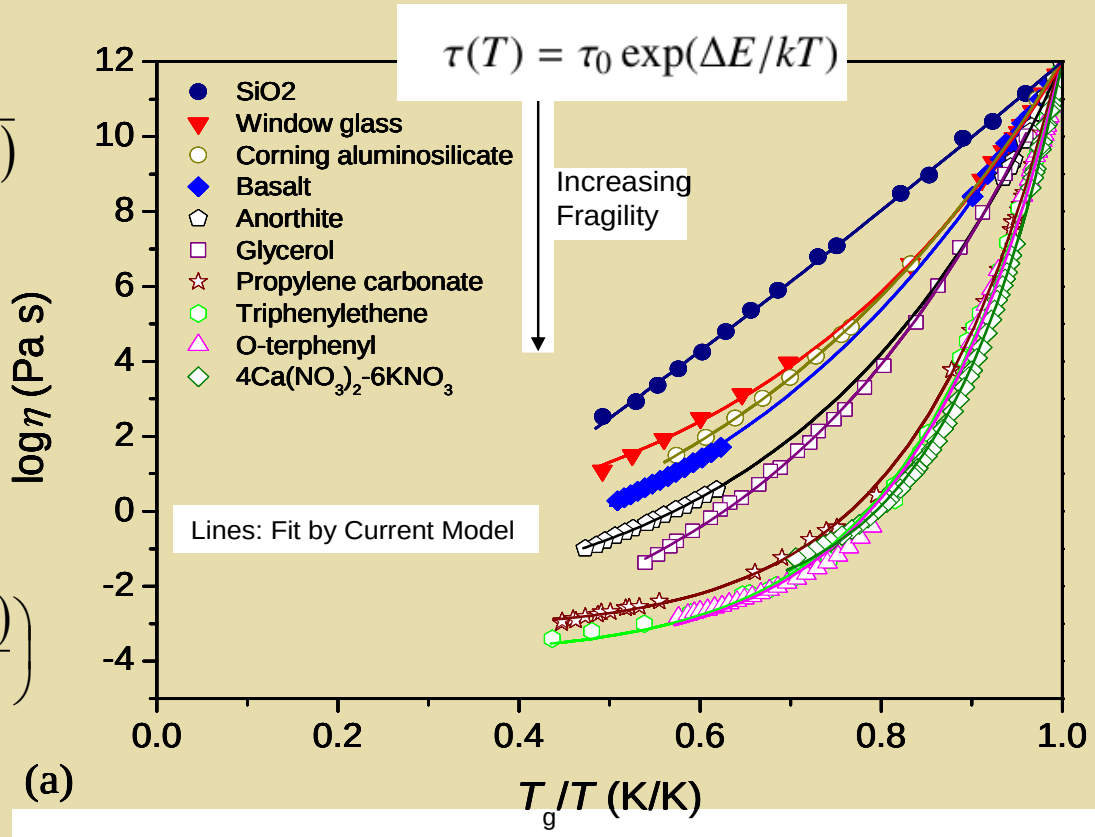


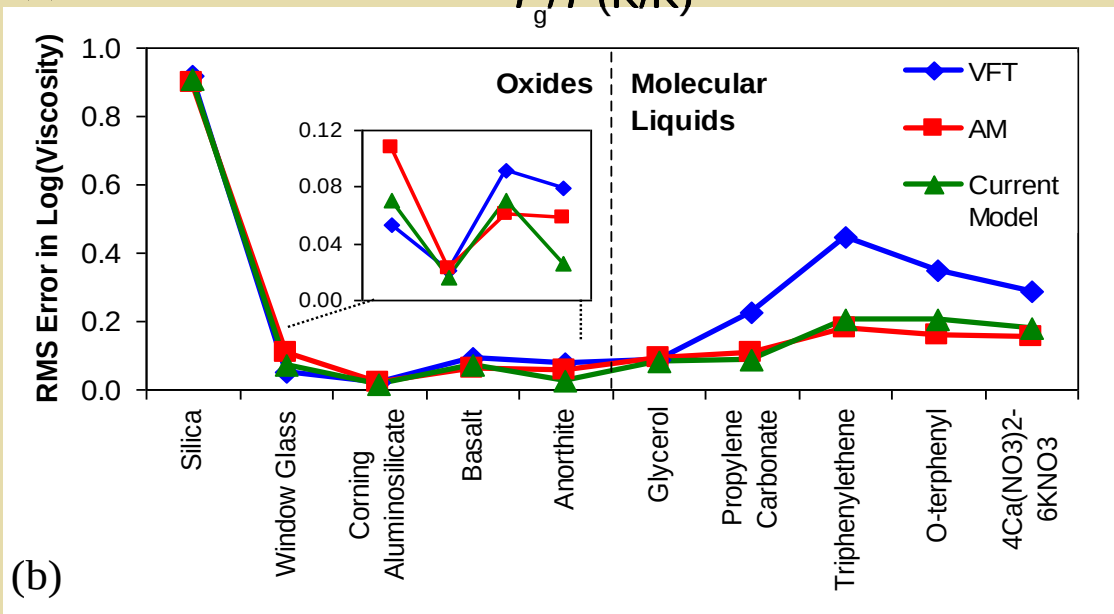
Naumis, Phys. Rev. E**71**, 026114 (2005).

$$\log_{10}\eta(T,x)=\log_{10}\eta_{\infty}(x)+\frac{B(x)}{TS_c(T,x)}$$

$$S_c(T,x)=f(T,x)Nk\ln\Omega$$

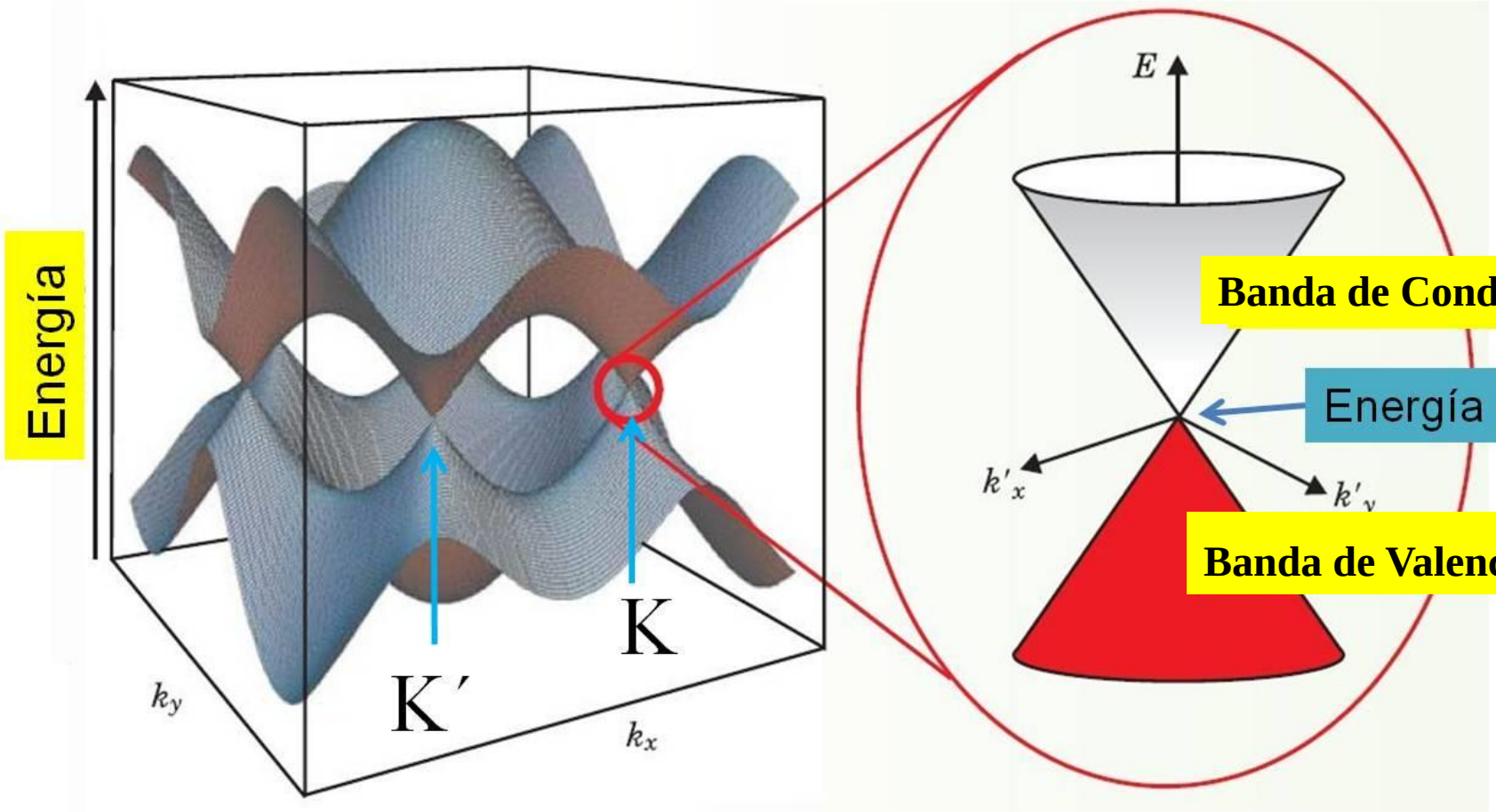
$$\log_{10}\eta(T,x)=\log_{10}\eta_{\infty}(x)+\frac{K(x)}{T}\exp\left(\frac{C(x)}{T}\right)$$





J.C. Mauro,et. al., PNAS, 2009

Later on, again we joined efforts but in flexibility of Graphene…



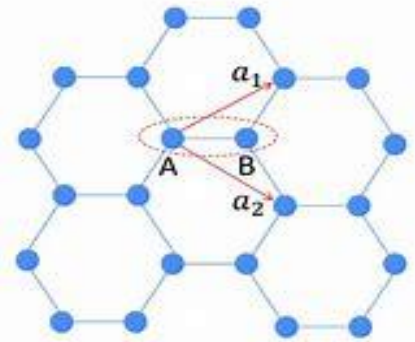
$$E(\vec{p}) = \pm v_F \left|\vec{p}\right|$$

$$E(\vec{p}) = \sqrt{p^2c^2 + m^2c^4}$$

$m \to 0;\ c \to v_F \approx 10^6 \mathrm{m/s}$

“Dirac like” Equation

$$\begin{pmatrix} 0 & H_{AB} \\ H_{AB}^{\dagger} & 0 \end{pmatrix} \begin{pmatrix} c_{A,i} \\ c_{B,i} \end{pmatrix} = \mathrm{E} \begin{pmatrix} c_{A,i} \\ c_{B,} \end{pmatrix}$$



$$-i\hbar v_F \begin{pmatrix} 0 & \frac{\partial}{\partial x} - i\frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} + i\frac{\partial}{\partial y} & 0 \end{pmatrix} \begin{pmatrix} \psi(r) \\ \chi(r) \end{pmatrix} = E \begin{pmatrix} \psi(r) \\ \chi(r) \end{pmatrix}$$

Electrons in graphene :
Dirac fermions

Semenoff, 1984
Haldane, 1988

- Near K point:
  - *Effective Hamiltonian* $H = v_F \vec{\sigma}.\vec{p}$

Pauli

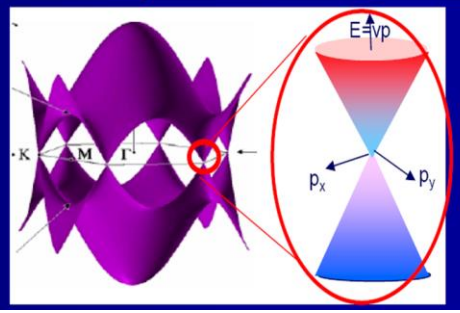
Dirac-Weyl equation: relativistic massless particle - Dirac fermions (“old” neutrino)

  - *linear dispersion*

$$E(\vec{q}) = \pm v_F \hbar |\vec{q}|,$$

$$\vec{q} = \vec{k} - \vec{K}_F, \quad v_F \approx 10^6 \,\mathrm{m/s} \sim \mathrm{c}/300$$

  - *Zero band mass*



Physica B 407 (2012) 2002–2008

Contents lists available at SciVerse ScienceDirect

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journal homepage: www.elsevier.com/locate/physb

Bending and flexural phonon scattering: Generalized Dirac equation for an electron moving in curved graphene

Richard Kerner [a,*], Gerardo G. Naumis [b], Wilfrido A. Gómez-Arias [b]

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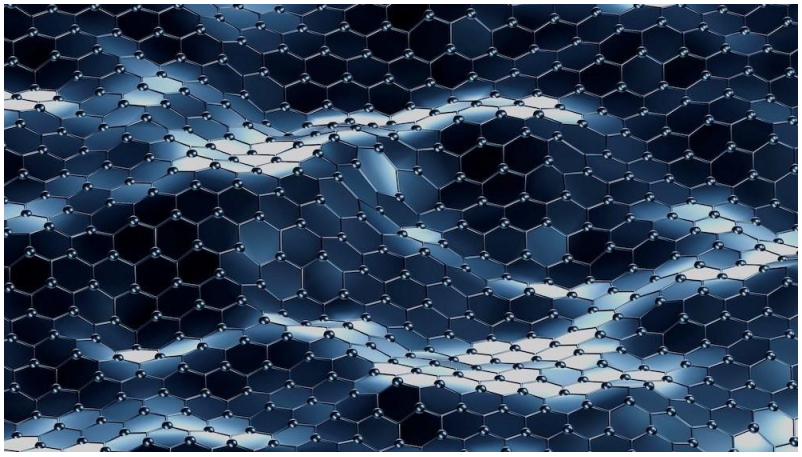
$$\hat{\tilde{H}}\Psi \sim [\tilde{\gamma}^x \tilde{\nabla}_x + \tilde{\gamma}^y \tilde{\nabla}_y]\Psi$$



$$\tilde{\nabla}_j \Psi = (\partial_j - eA_j)\Psi + \tilde{\Gamma}^m_{jk}\tilde{g}^{ki}\tilde{\Sigma}_{mi}\Psi, \tag{5}$$

where the Christoffel symbols $\tilde{\Gamma}^m_{jk}$ are defined as usual, by means of the modified metric:

$$\tilde{\Gamma}^i_{jk} = \tfrac{1}{2}\tilde{g}^{im}[\partial_j \tilde{g}_{mk} + \partial_k \tilde{g}_{jm} - \partial_m \tilde{g}_{jk}] \tag{6}$$

and $\tilde{\Sigma}_{mk}$ is the matrix-valued anti-symmetric tensor defined by means of the modified gamma-matrices:

$$\tilde{\Sigma}_{mk} = \tfrac{1}{8}[\tilde{\gamma}_m \tilde{\gamma}_k - \tilde{\gamma}_k \tilde{\gamma}_m]. \tag{7}$$

$$\hat{\tilde{H}} \sim \hat{H}_0 + \sigma_z(\overrightarrow{\text{grad}}\, f)\cdot(\vec{\nabla}) - (\overrightarrow{\text{grad}}\, f \cdot \vec{\sigma})(\overrightarrow{\text{grad}}\, f \cdot \vec{\nabla}) + \tfrac{1}{8}\,\vec{\sigma}\cdot\overrightarrow{\text{grad}}[(\partial_x f)^2 + (\partial_y f)^2] - \tfrac{1}{4}[\vec{\sigma}\cdot\overrightarrow{\text{grad}}\, f]\Delta f.$$

PRL 118, 046601 (2017) PHYSICAL REVIEW LETTERS week ending 27 JANUARY 2017

Flexural-Phonon Scattering Induced by Electrostatic Gating in Graphene

Tue Gunst,* Kristen Kaasbjerg, and Mads Brandbyge
Department of Micro- and Nanotechnology (DTU Nanotech), Center for Nanostructured Graphene (CNG), Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark
(Received 20 September 2016; published 27 January 2017)

Nanoscale

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Cite this: *Nanoscale*, 2016, **8**, 9822

Controlling the ripple density and heights: a new way to improve the electrical performance of CVD-grown graphene†

Won-Hwa Park,‡§[a] Insu Jo,§[b] Byung Hee Hong*[b] and Hyeonsik Cheong*[a]

IOP Publishing Journal of Physics: Condensed Matter
J. Phys.: Condens. Matter **26** (2014) 185301 (14pp) doi:10.1088/0953-8984/26/18/185301

Optical conductivity of curved graphene

A J Chaves[1], T Frederico[1], O Oliveira[1, 2], W de Paula[1, 3] and M C Santos[2]

Experimental investigation of surface morphology of a chemical vapor deposition-grown graphene monolayer mediating with a gap-plasmonic system and the related ripple shape study

Cite as: J. Appl. Phys. **124**, 223101 (2018); https://doi.org/10.1063/1.5066042
Submitted: 12 October 2018 • Accepted: 24 November 2018 • Published Online: 13 December 2018

Won-Hwa Park, Minjung Kim, Jaebum Choo, et al.

www.nature.com/scientificreports

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From curved spacetime to spacetime-dependent local unitaries over the honeycomb and triangular Quantum Walks

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Accepted: 15 July 2019
Published online: 29 July 2019

Pablo Arrighi[1], Giuseppe Di Molfetta[2], Ivan Marquez-Martin[2] & Armando Perez[3]

Eur. Phys. J. C (2022) 82:8
https://doi.org/10.1140/epjc/s10052-021-09938-4

THE EUROPEAN PHYSICAL JOURNAL C

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Regular Article - Theoretical Physics

Aspects of the polynomial affine model of gravity in three dimensions

With focus in the cosmological solutions

PHYSICAL REVIEW LETTERS **121,** 036403 (2018)

Editors' Suggestion

Quantum Holography in a Graphene Flake with an Irregular Boundary

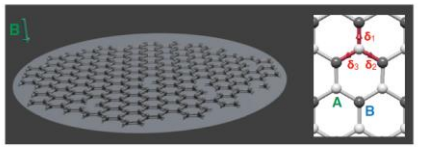
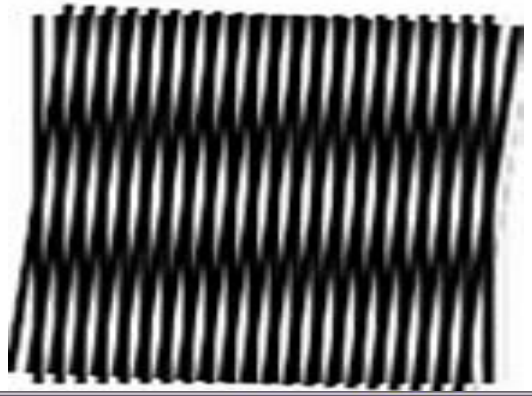
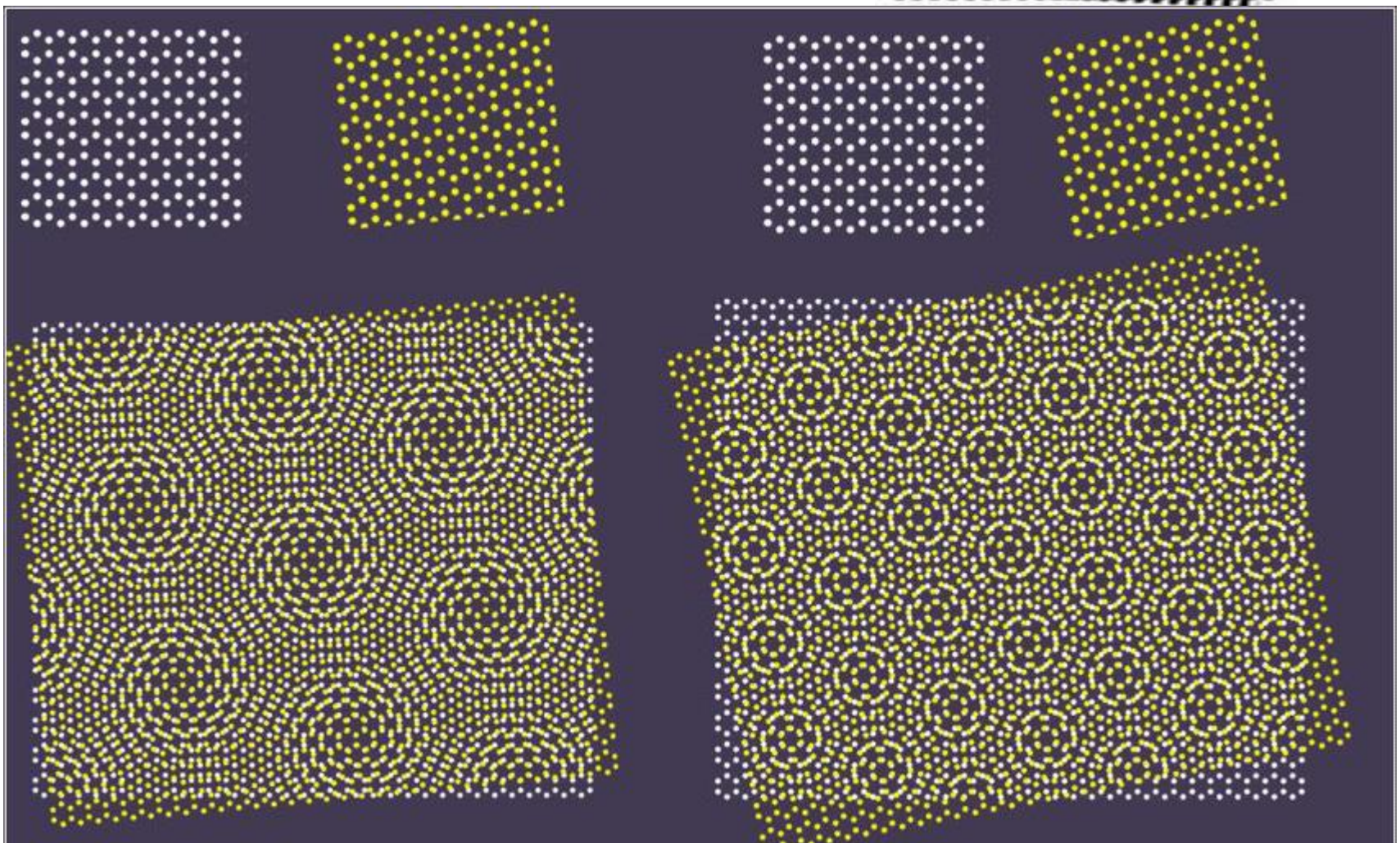


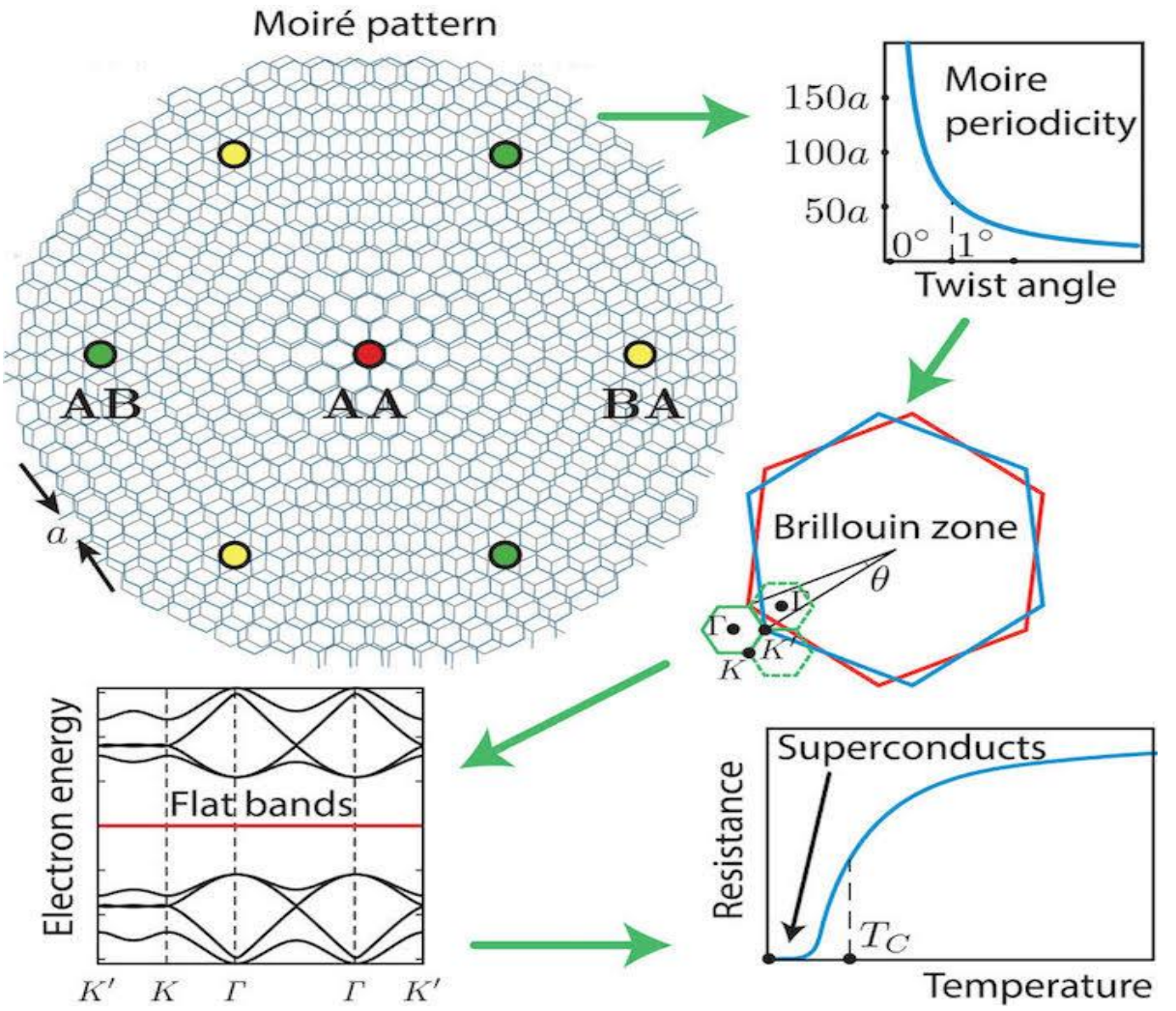
FIG. 1. Schematic depiction of the proposed device. Irregular shaped graphene flake in applied magnetic field B forms the $(0+1)$-dimensional many-body system equivalent to a black hole in $(1+1)$ anti–de Sitter space. Inset: lattice structure of graphene with A and B sublattices marked and nearest neighbor vectors denoted by $\boldsymbol{\delta}_j$.

Twistronics= Girotrónica





Moiré patterns and superconductivity….



$$L(\theta) = a_0/2\sin\theta/2$$

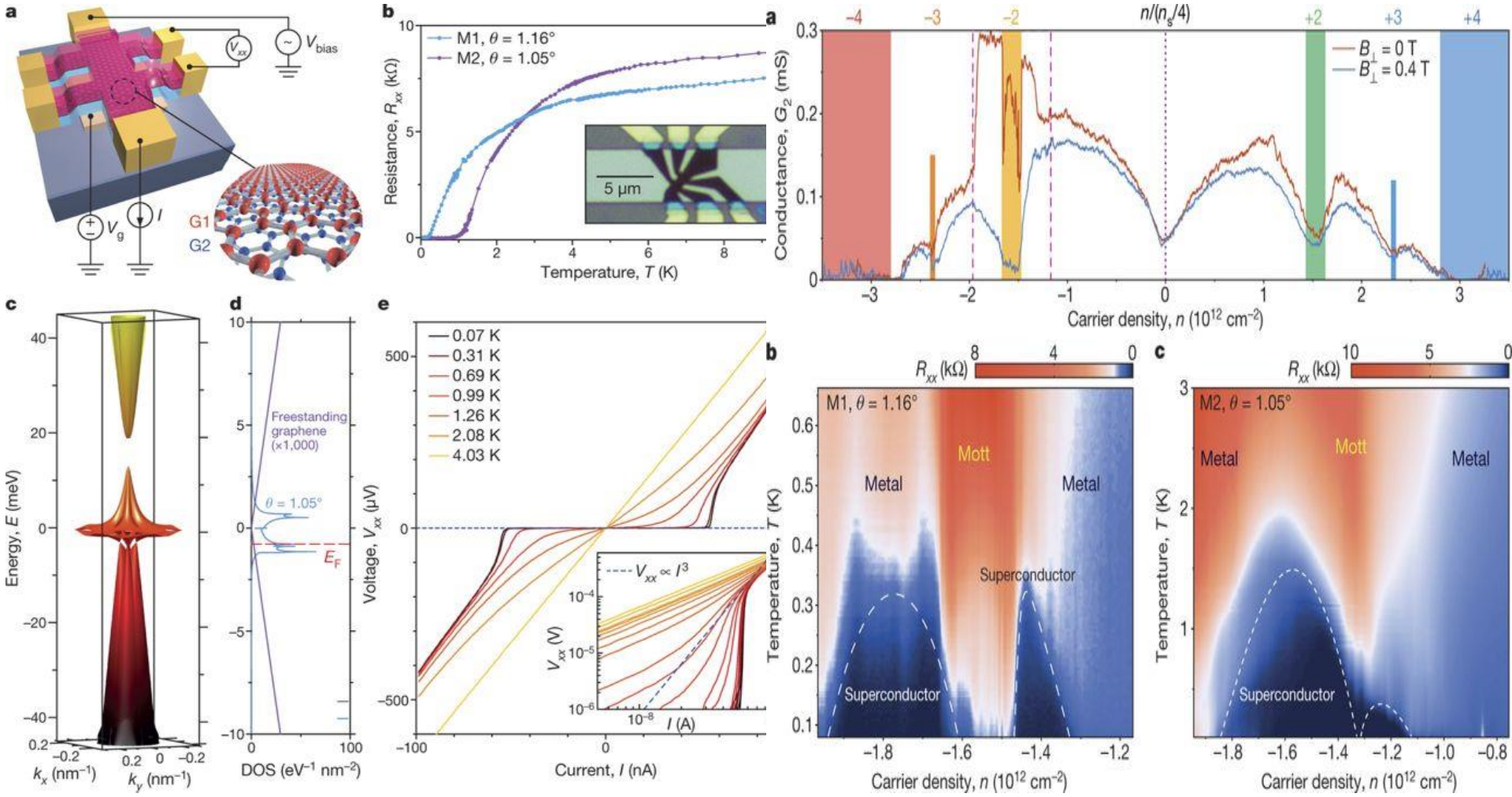
$$k_\theta = 2k_D\sin(\theta/2)$$

$$k_D = 4\pi/(3a_0)$$

$$\boldsymbol{a}_{1,2} = \frac{4\pi}{3k_\theta}\left(\pm\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \qquad \boldsymbol{b}_{1,2} = \boldsymbol{q}_{2,3} - \boldsymbol{q}_1 = k_\theta\left(\pm\frac{\sqrt{3}}{2}, \frac{3}{2}\right)$$

Unconventional superconductivity in magic-angle graphene superlattices

Cao,…, Jarrillo-Herrero, Nature, 556, pages 43–50 (05 April 2018)



R. Bistritzer and A. H. MacDonald, "Moire bands in twisted double-layer graphene," *Proceedings of the National Academy of Sciences*, vol. 108, pp. 12233–12237, jul 2011.

Superconductivity of TBG
Jarrillo-Herrero, et. al. , Nature (2018)

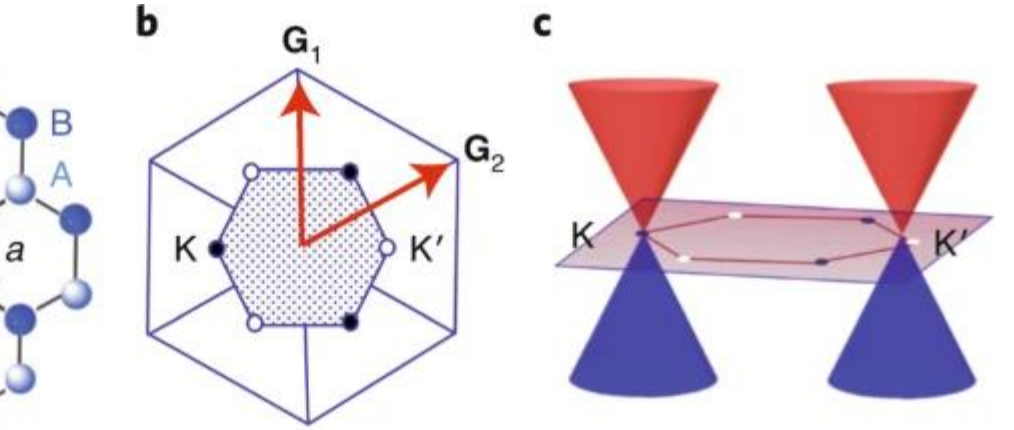
Chiral Model (4x4 Operator)
Tarnopolsky, Jura, Vishnawatan , PRL 2019

Magic angle hierarchy in twisted graphene multilayers
E. Khalaf, A.J. Kruchkov, G. Tarnopolsky, and A. Vishwanath
Phys. Rev. B 100, 085109 (2019)

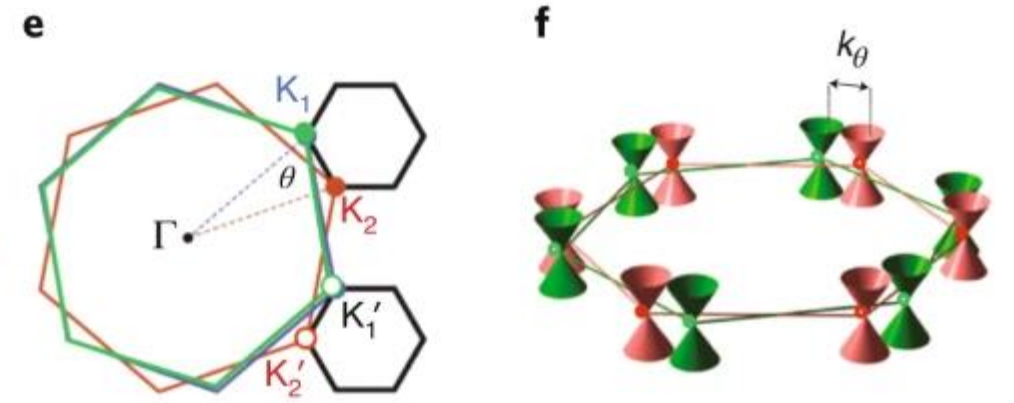
Model 2x2, PRB (2021)

Electric field–tunable superconductivity in alternating-twist magic-angle trilayer graphene, *Science*, 12 Mar 2021, **Large Pauli Limit Violation and Reentrant Superconductivity** **Cao, Park, Jarrillo-Herrero**, arXiv:2103.12083v1 Marzo (2021)

Modelo de Bistrizer-Mac Donald (2011)



$$H_+ = \begin{bmatrix} H_{UU} & H_{UD} \\ H_{DU} & H_{DD} \end{bmatrix}$$



$$\sigma_{\theta/2} = e^{-i\frac{\theta}{4}\sigma_z}(\sigma_x, \sigma_y)e^{+i\frac{\theta}{4}\sigma_z}$$

$$H_{UU} = v_F(-i\nabla - \mathbf{K^U}) \cdot \sigma_{\theta/2}$$

$$H_{DD} = v_F(-i\nabla - \mathbf{K^D}) \cdot \sigma_{-\theta/2}$$

$$H_{UD} = T_0(r)\sigma^0 + T_{AB}(r)\sigma^+ + T_{BA}(r)\sigma^-$$

R. Bistritzer and A. H. MacDonald, "Moire bands in twisted double-layer graphene," *Proceedings of the National Academy of Sciences*, vol. 108, pp. 12233–12237, jul 2011.

Andrei, Mac Donald, Nature Materials volume 19, pages1265–1275(2020)

PHYSICAL REVIEW LETTERS **122,** 106405 (2019)

Editors' Suggestion

Origin of Magic Angles in Twisted Bilayer Graphene

Grigory Tarnopolsky, Alex Jura Kruchkov,* and Ashvin Vishwanath
Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

AA tunelling set 0

$$\Phi(\mathbf{r}) = (\psi_1, \psi_2, \chi_1, \chi_2)^{\mathrm{T}} \qquad \mathcal{H}\Phi_{\mathbf{k}}(\mathbf{r}) = \varepsilon_0(\mathbf{k})\Phi_{\mathbf{k}}$$

$$\mathcal{H} = \begin{pmatrix} 0 & D^*(-r) \\ D(r) & 0 \end{pmatrix}$$

where the zero-mode operator is,

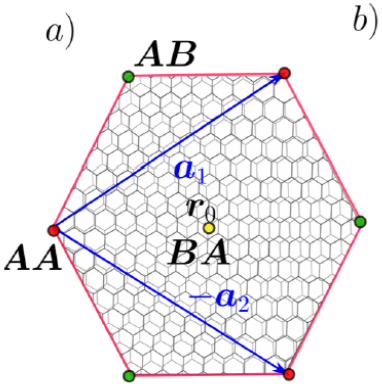
$$D(r) = \begin{pmatrix} -i\bar{\partial} & \alpha U(r) \\ \alpha U(-r) & -i\bar{\partial} \end{pmatrix}$$

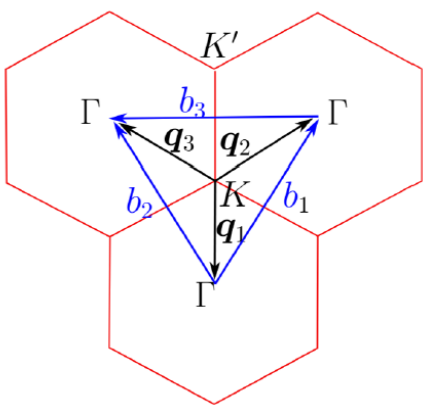
from where,

$$D^*(-r) = \begin{pmatrix} -i\partial & \alpha U^*(-r) \\ \alpha U^*(r) & -i\partial \end{pmatrix}$$

and $\bar{\partial} = \partial_x + i\partial_y$, $\partial = \partial_x - i\partial_y$. The potential is

$$U(\boldsymbol{r}) = e^{-i\boldsymbol{q}_1\cdot\boldsymbol{r}} + e^{i\phi}e^{-i\boldsymbol{q}_2\cdot\boldsymbol{r}} + e^{-i\phi}e^{-i\boldsymbol{q}_3\cdot\boldsymbol{r}}$$





$$\alpha = \frac{w_1}{v_0 k_\theta}$$

Angle and energy=coupling constant

$$k_\theta = 2k_D \sin(\theta/2)$$

$$\phi = \frac{2\pi}{3}$$

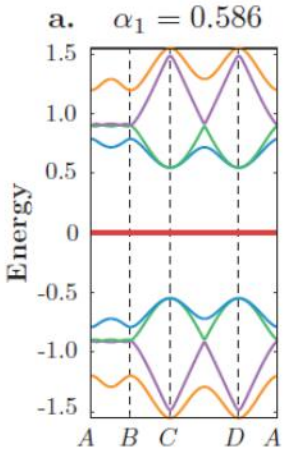
Naumis, L. Navarro,E. Aguilar, A. Espinosa, PRB 2021

$$\mathcal{H}^2 = \begin{pmatrix} D^*(-r)D(r) & 0 \\ 0 & D(r)D^*(-r) \end{pmatrix}$$

Navarro, Naumis, Phys. Rev. B (2022)
Navarro, Naumis, Phys. Rev. B (2023)

Supersymmetry leads to flexible phonon modes!

$$H^2 = \begin{pmatrix} -\nabla^2 + \alpha^2|U(-\boldsymbol{r})|^2 & \alpha A^\dagger(\boldsymbol{r}) \\ \alpha A(\boldsymbol{r}) & -\nabla^2 + \alpha^2|U(\boldsymbol{r})|^2 \end{pmatrix}$$

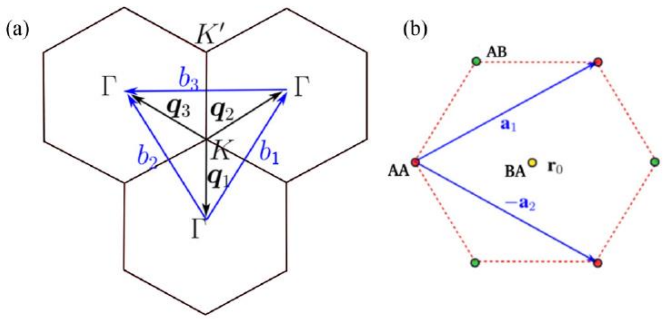


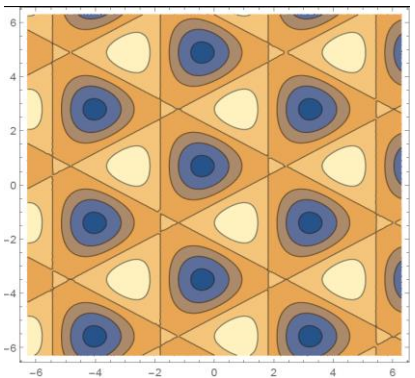
$$A(\boldsymbol{r}) = -i\sum_{\mu=1}^{3} e^{i\boldsymbol{q}_\mu\cdot\boldsymbol{r}}(2\hat{\boldsymbol{q}}_\mu^{\perp}\cdot\boldsymbol{\nabla} - 1)$$

Non-Abelian Gauge

$$|U(\boldsymbol{r})|^2 = 3+2\cos(\boldsymbol{b}_1\cdot\boldsymbol{r}-\phi)+2\cos(\boldsymbol{b}_2\cdot\boldsymbol{r}+\phi)+2\cos(\boldsymbol{b}_3\cdot\boldsymbol{r}+2\phi)$$

Confinement Potential: Moiré Triangular Lattice





- CONCLUSION

1) Richard: thanks for all these years teaching us how to do research and teach and plus all sort of things and jokes.

2) Remark his huge impact in third world science