Mesoscopic physics: From low-energy nuclear [1] to relativistic [2] high-energy analogies

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School of Physics, Georgia Institute of Technology

[1] Ch. 4 in **“Metal Clusters”**,
edited by W. Ekardt (John-Wiley, New York, 1999) pp. 145 – 180;

Rep. Prog. Phys. **70** (2007) pp. 2067-2148

[2] PRB **89,** 035432 (2014); PRB **87,** 165431 (2013)

NMP14, 5-9 May 2014

Supported by the U.S. DOE (FG05-86ER45234)

Mesoscopics:

"The area of condensed-matter physics that covers the transition regime between macroscopic objects and the microscopic, atomic world."

TU Delft course

Finite-size condensed-matter nanosystems
(small systems and transition to the bulk)

Nuclear analogies (nonrelativistic electrons/ Schrödinger equation):
(3D) metal clusters, metal grains,fullerenes;
(2D) quantum billiards, quantum dots; quantum islands;
(1D) quantum-point contacts, nanowires, quantum rings, interferometers

Particle-physics analogies (relativistic electrons/ Dirac equation):
Graphene-based nanosystems:
(2D) graphene quantum dots;
(1D) uniform and segmented graphene nanoribbons (junctions), graphene polygonal rings

FIRST PART

Some examples (among many, e.g., random matrix theory) of nuclear analogies

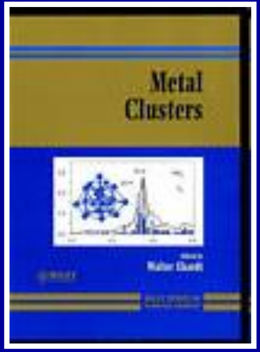
(from personal experience)

In this talk: Emphasis on broader qualitative aspects and not on mathematical theoretical formulation

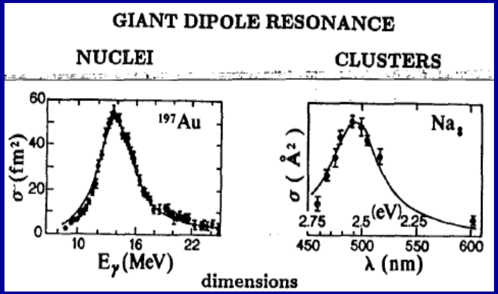
Collaborators: Uzi Landman, Igor Romanovsky, Yuesong Li, Ying Li, Leslie Baksmaty, R.N. Barnett

Three (among others) major nuclear aspects:

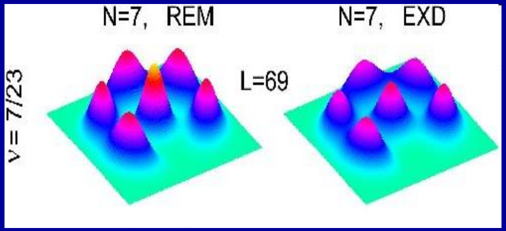
- *Electronic shells/deformation/fission*
  (via Strutinsky/ Shell correction approach) in metal clusters
  [see, e.g., Yannouleas, Landman, Barnett, in “Metal Clusters”,
  edited by W. Ekardt, John-Wiley, 1999]



- *Surface plasmons/Giant resonances*
  (via matrix RPA/LDA) in metal clusters
  [see, e.g., Yannouleas, Broglia, Brack, Bortignon,
  PRL **63,** 255 (1989)]



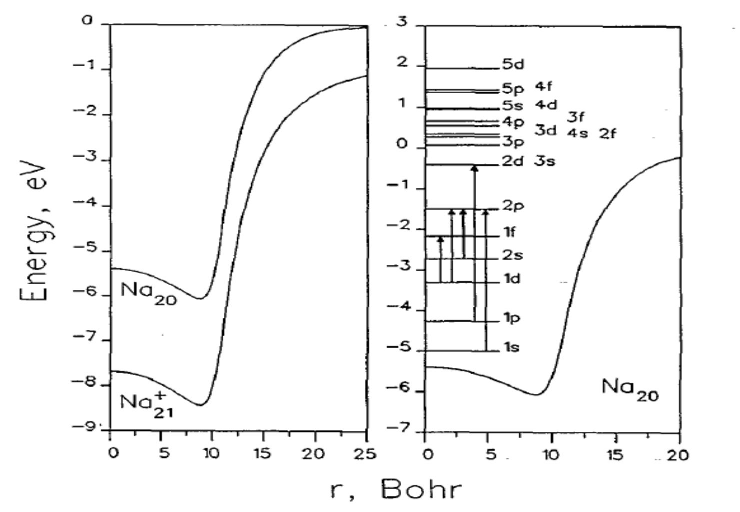
- *Strongly correlated states (Quantum crystals/Wigner molecules/dissociation)*
  in 2D semiconductor quantum dots and
  ultracold bosonic traps via
  symmetry breaking/symmetry restoration
  in conjunction with exact diagonalization (full CI)
  [see, e.g., Yannouleas, Landman,
  Rep. Prog. Phys. **70,** 2067 (2007)]

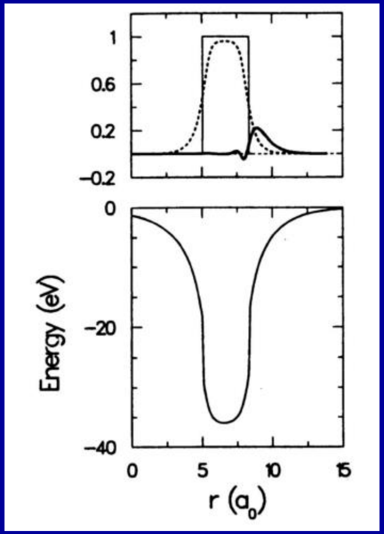


- *Electronic shells/ magic numbers/ deformation/ fission* in metal clusters
- *Surface plasmons/Giant resonances* in metal clusters

The physics of free nonrelativistic electrons confined in a central potential, like atomic nuclei

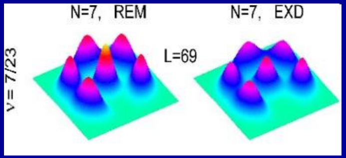
(conservation of symmetries/ independent particle model/ delocalized electrons)

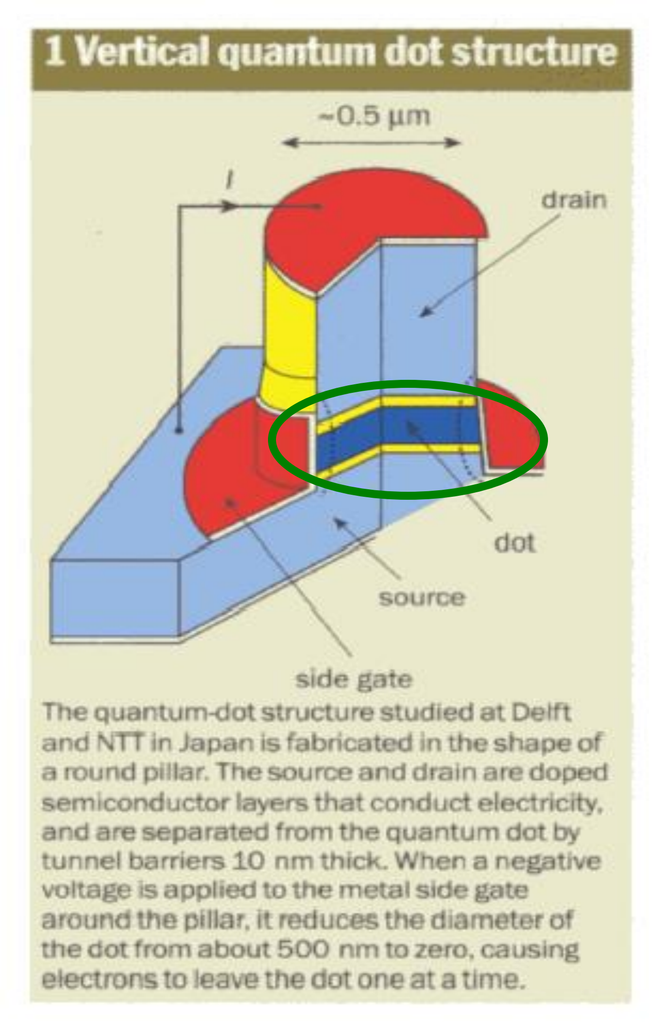




- *Strongly correlated states (Quantum crystals/Wigner molecules/dissociation)* in 2D semiconductor quantum dots

No central potential/ electron localization (relative to each other) due to strong Coulomb repulsion/ mean-filed with broken symmetries





1 Vertical quantum dot structure

The quantum-dot structure studied at Delft and NTT in Japan is fabricated in the shape of a round pillar. The source and drain are doped semiconductor layers that conduct electricity, and are separated from the quantum dot by tunnel barriers 10 nm thick. When a negative voltage is applied to the metal side gate around the pillar, it reduces the diameter of the dot from about 500 nm to zero, causing electrons to leave the dot one at a time.

Vertical QD (Delft)

Electrostatic confinement

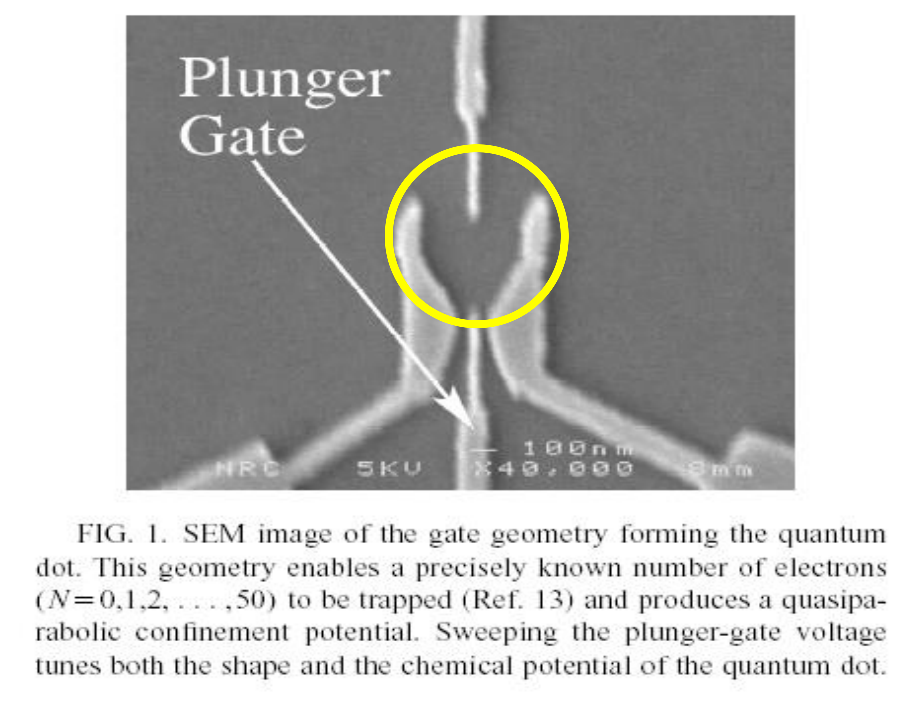
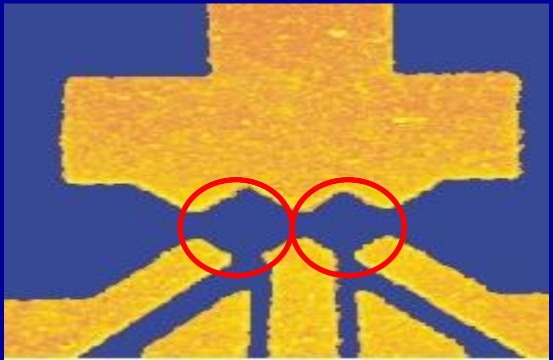
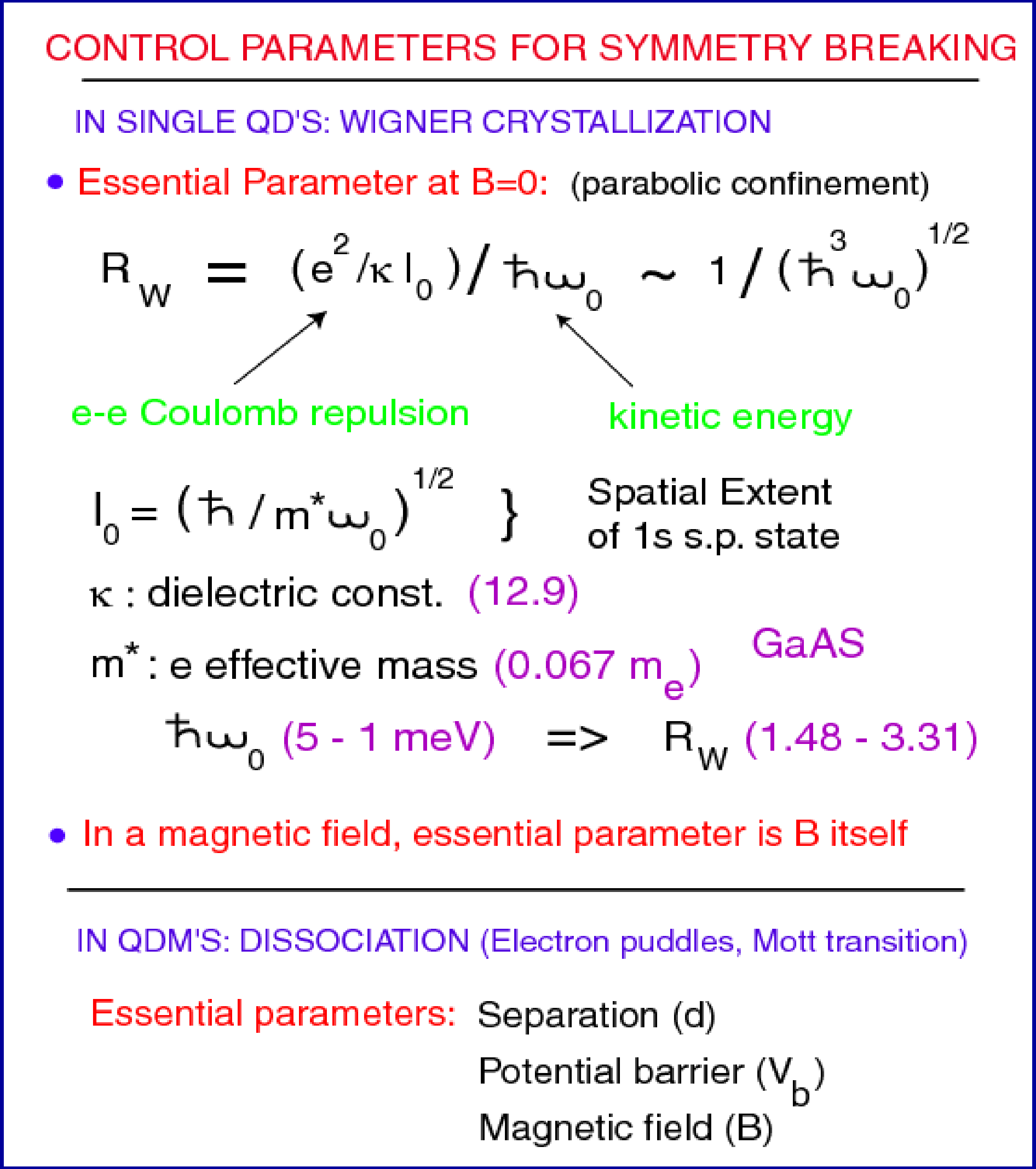


FIG. 1. SEM image of the gate geometry forming the quantum dot. This geometry enables a precisely known number of electrons ($N=0,1,2, \ldots ,50$) to be trapped (Ref. 13) and produces a quasiparabolic confinement potential. Sweeping the plunger-gate voltage tunes both the shape and the chemical potential of the quantum dot.

Lateral QD (Ottawa)



Lateral QD Molecule (Delft)



CONTROL PARAMETERS FOR SYMMETRY BREAKING

IN SINGLE QD'S: WIGNER CRYSTALLIZATION

- Essential Parameter at B=0: (parabolic confinement)

$$R_W = (e^2/\kappa l_0)/\hbar\omega_0 \sim 1/(\hbar^3\omega_0)^{1/2}$$

e-e Coulomb repulsion

kinetic energy

$$l_0 = (\hbar / m^*\omega_0)^{1/2} \quad \}$$ Spatial Extent of 1s s.p. state

κ : dielectric const. (12.9)

m^* : e effective mass ($0.067\ m_e$) GaAS

$\hbar\omega_0$ (5 - 1 meV) => R_W (1.48 - 3.31)

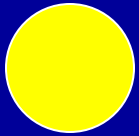
- In a magnetic field, essential parameter is B itself

IN QDM'S: DISSOCIATION (Electron puddles, Mott transition)

Essential parameters: Separation (d)
Potential barrier (V_b)
Magnetic field (B)

$$R_\delta = gm/(2\pi\hbar^2)$$

Neutral bosons



Circular external confinement

$B = 0$

Wigner molecule in a 2D circular QD.

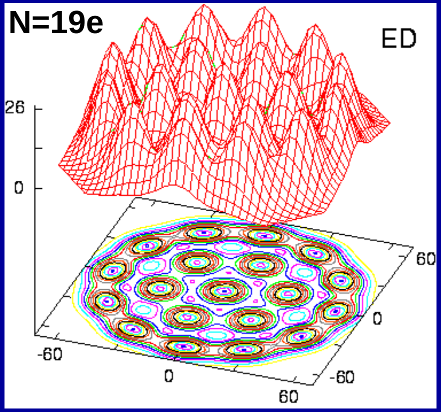
Electron density (ED) from

Unrestricted Hartree-Fock (UHF).

Symmetry breaking (localized orbitals).

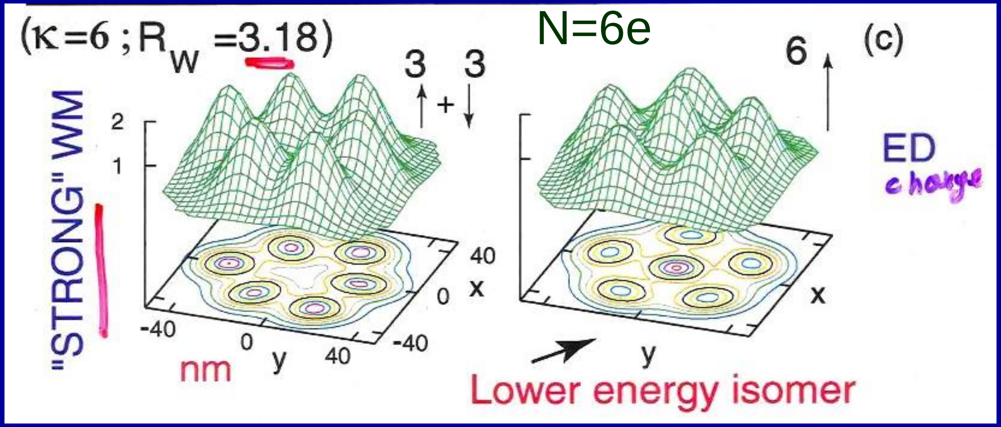
Concentric polygonal rings

$R_W = 5$



Concentric rings: (1,6,12)

Y&L,
PRB 68, 035325 (2003)



Concentric rings: (0,6) left, (1,5) right

Y&L, PRL 82, 5325 (1999)

Exact electron densities are circular!
No symmetries are broken!
(N, small, large?)

Restoration of symmetry ➡ Quantum crystal

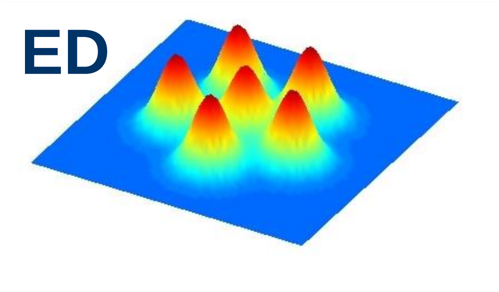
Rotating Boson Molecules (Circular trap)

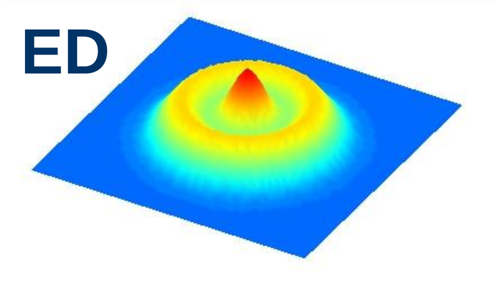
Ground states: Energy, angular momentum and probability densities.

$R_\delta = 50$

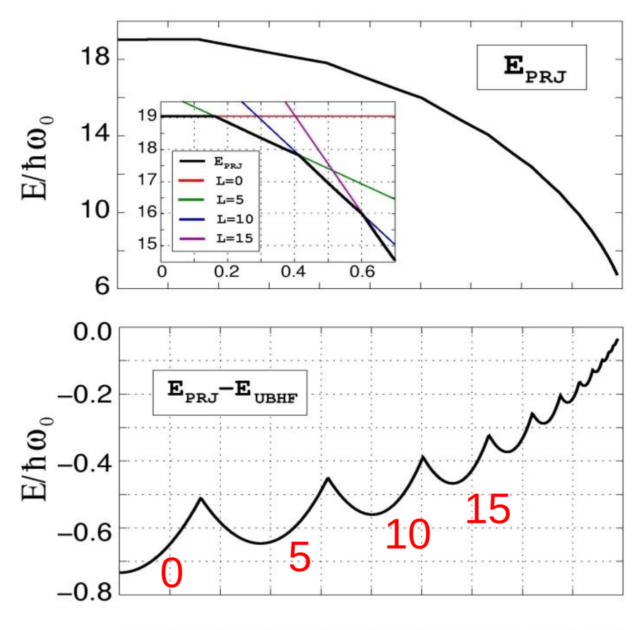
$R_W = 10$

Probability densities

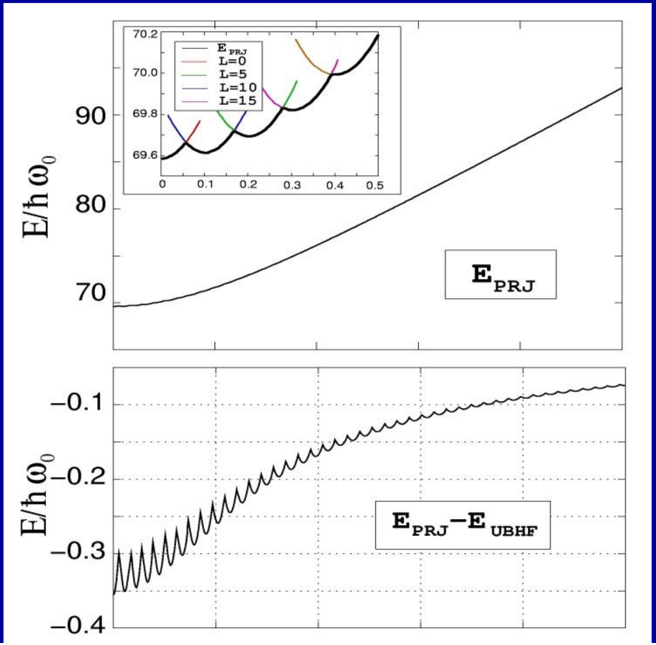


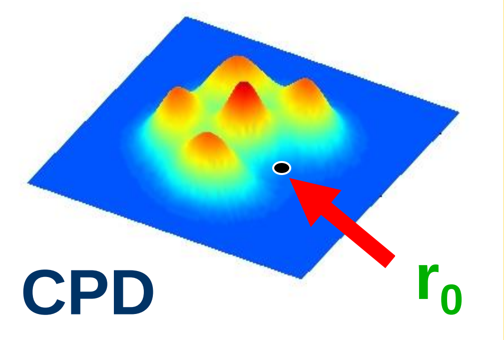


Rotating Frame



Magnetic Field





The hidden crystalline structure in the projected function can be revealed through the use of conditional probability density (CPD).

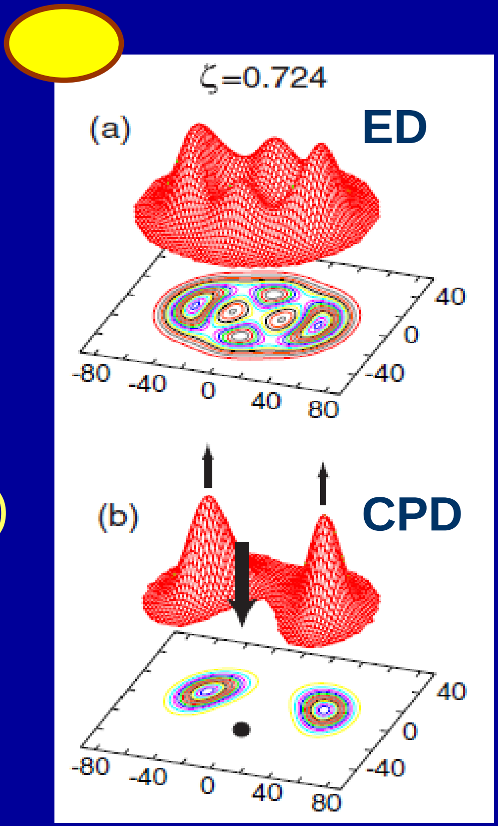
$$\rho(\mathbf{r}|\mathbf{r_0}) = \langle\Phi|\sum_{i\neq j}\delta(\mathbf{r}_i - \mathbf{r})\delta(\mathbf{r}_j - \mathbf{r}_0)|\Phi\rangle / \langle\Phi|\Phi\rangle$$

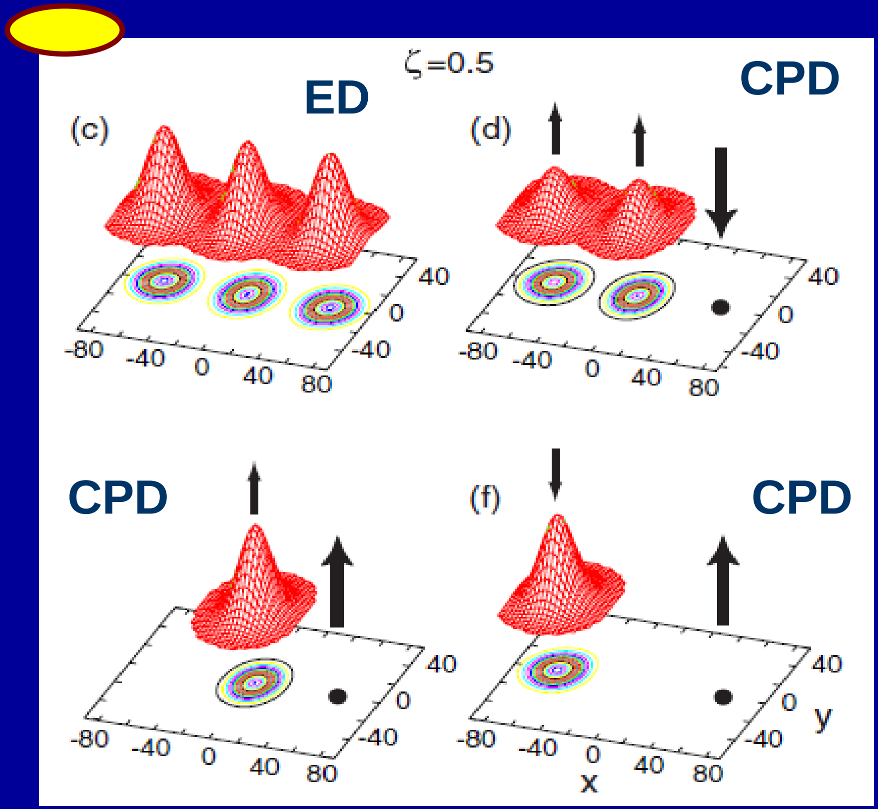
Three electron anisotropic QD

Method: ***Exact Diagonalization (EXD)***

Anisotropic confinement

Electron Density (ED)





(spin resolved) Conditional Probability Distribution (CPD)

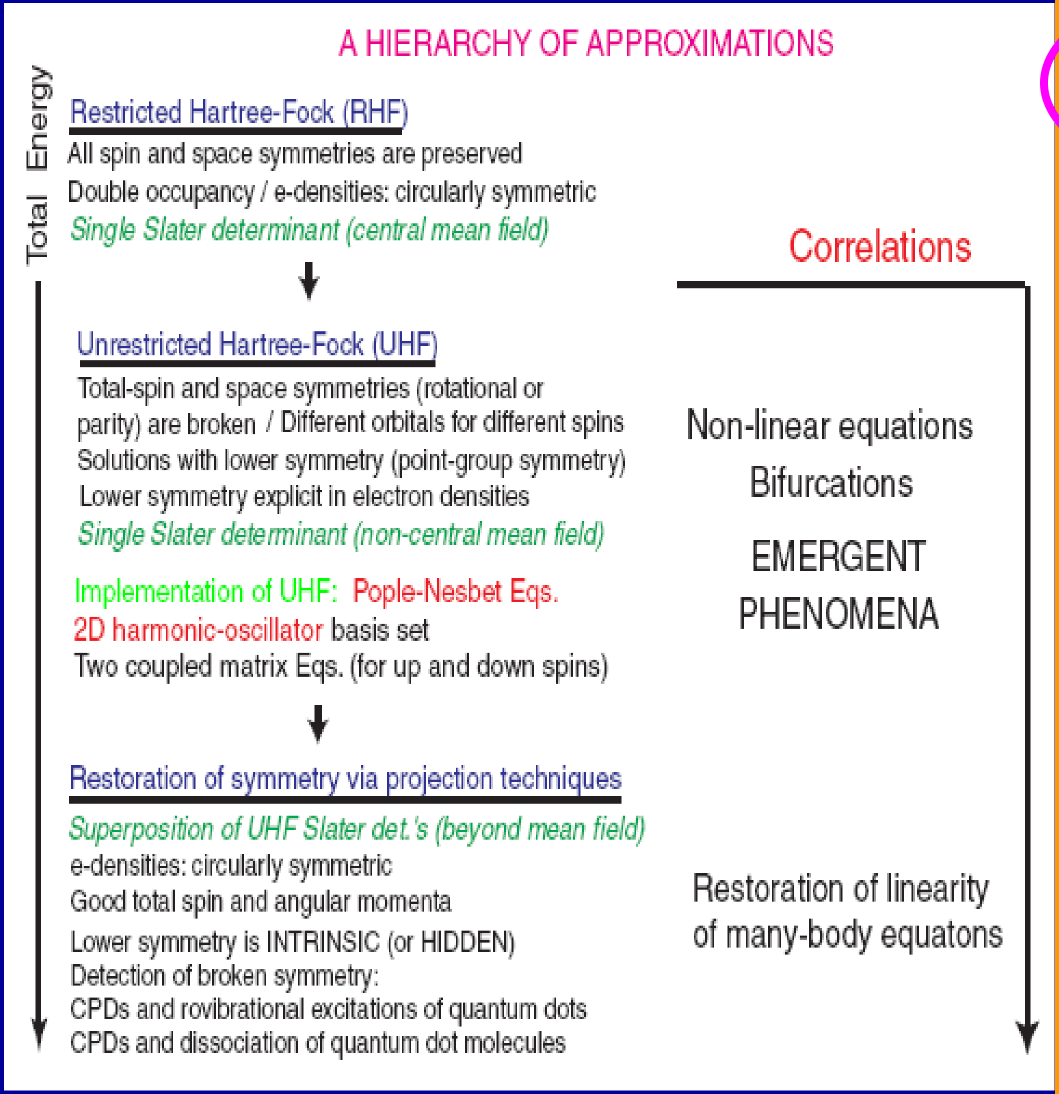
Yuesong Li, Y&L, Phys. Rev. B **76,** 245310 (2007)

EXD wf ~ $|\downarrow\uparrow\uparrow> - |\uparrow\uparrow\downarrow>$

Entangled three-qubit W-states

WAVE-FUNCTION BASED APPROACHES

TWO-STEP METHOD



A HIERARCHY OF APPROXIMATIONS

Total Energy

Restricted Hartree-Fock (RHF)

All spin and space symmetries are preserved
Double occupancy / e-densities: circularly symmetric
Single Slater determinant (central mean field)

Correlations

Unrestricted Hartree-Fock (UHF)

Total-spin and space symmetries (rotational or parity) are broken / Different orbitals for different spins
Solutions with lower symmetry (point-group symmetry)
Lower symmetry explicit in electron densities
Single Slater determinant (non-central mean field)

Non-linear equations
Bifurcations

EMERGENT
PHENOMENA

Implementation of UHF: Pople-Nesbet Eqs.
2D harmonic-oscillator basis set
Two coupled matrix Eqs. (for up and down spins)

Restoration of symmetry via projection techniques

Superposition of UHF Slater det.'s (beyond mean field)
e-densities: circularly symmetric
Good total spin and angular momenta
Lower symmetry is INTRINSIC (or HIDDEN)
Detection of broken symmetry:
CPDs and rovibrational excitations of quantum dots
CPDs and dissociation of quantum dot molecules

Restoration of linearity
of many-body equatons

EXACT DIAGONALIZATION

(Full Configuration Interaction)

When possible (small N):
High numerical accuracy

Physics less transparent compared to "THE TWO-STEP"

Pair correlation functions, CPDs

Yannouleas and Landman, Rep. Prog. Phys. ***70****, 2067 (2007)*

RESOLUTION OF SYMMETRY DILEMMA:

RESTORATION OF BROKEN SYMMETRY BEYOND MEAN FIELD (Projection)!

- Per-Olov Löwdin

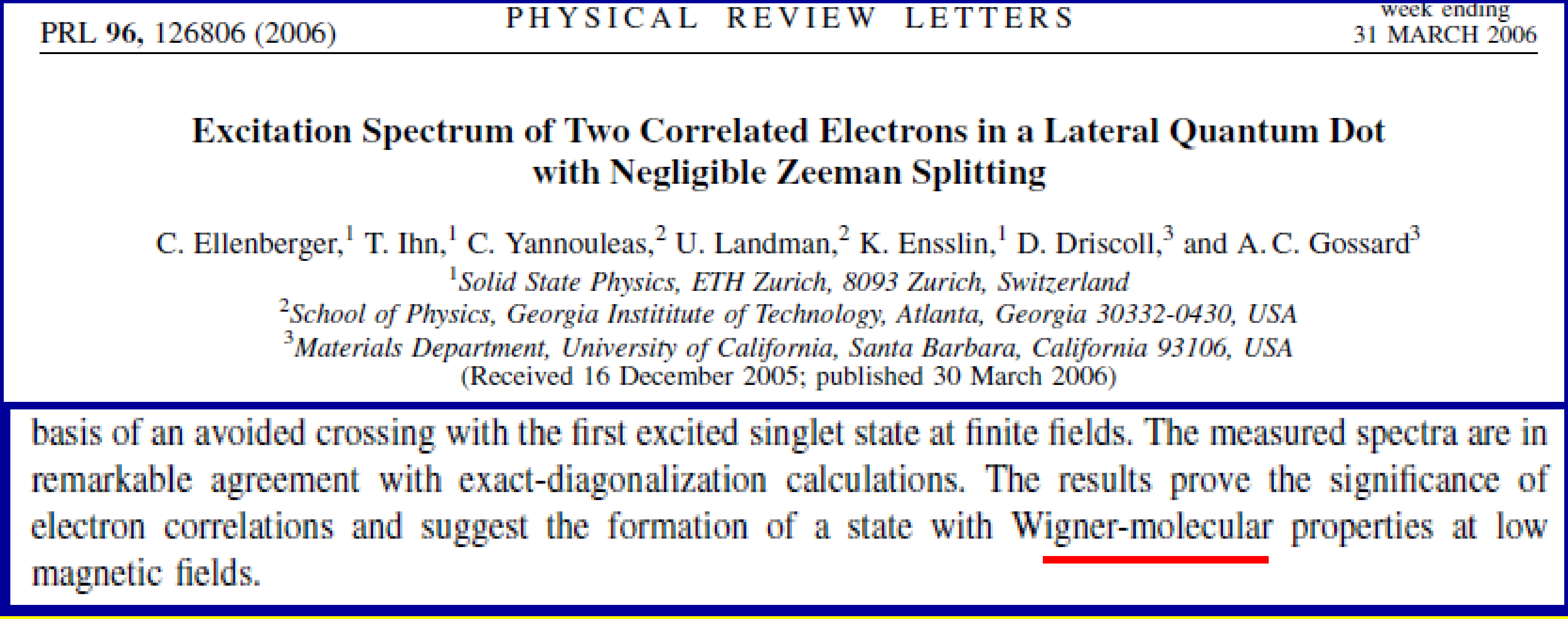
  (Chemistry - Spin)
- R.E. Peierls and J. Yoccoz

  (Nuclear Physics – *L, rotations*)

Ch. 11 in the book by P. Ring and P. Schuck

Note: Example in 2D

Yannouleas, Landman, Rep. Prog. Phys. **70,** 2067 (2007)



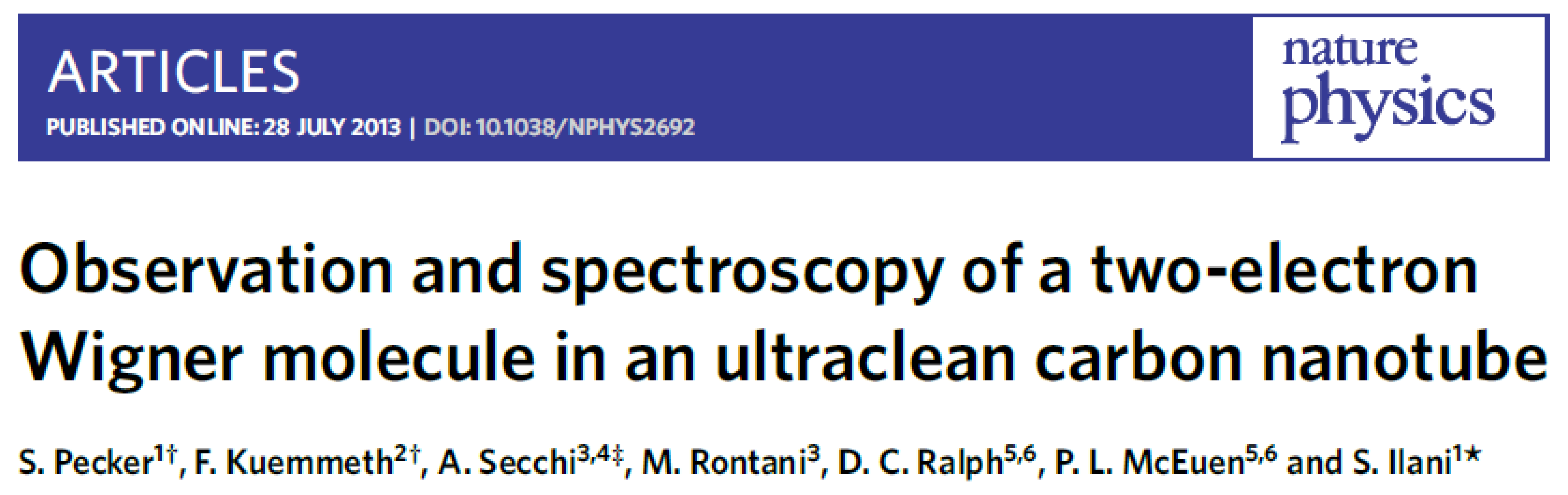
PRL 96, 126806 (2006) PHYSICAL REVIEW LETTERS week ending 31 MARCH 2006

Excitation Spectrum of Two Correlated Electrons in a Lateral Quantum Dot with Negligible Zeeman Splitting

C. Ellenberger,[1] T. Ihn,[1] C. Yannouleas,[2] U. Landman,[2] K. Ensslin,[1] D. Driscoll,[3] and A. C. Gossard[3]

[1] *Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland*
[2] *School of Physics, Georgia Instititute of Technology, Atlanta, Georgia 30332-0430, USA*
[3] *Materials Department, University of California, Santa Barbara, California 93106, USA*
(Received 16 December 2005; published 30 March 2006)

basis of an avoided crossing with the first excited singlet state at finite fields. The measured spectra are in remarkable agreement with exact-diagonalization calculations. The results prove the significance of electron correlations and suggest the formation of a state with Wigner-molecular properties at low magnetic fields.



ARTICLES

PUBLISHED ONLINE: 28 JULY 2013 | DOI: 10.1038/NPHYS2692

nature physics

Observation and spectroscopy of a two-electron Wigner molecule in an ultraclean carbon nanotube

S. Pecker[1†], F. Kuemmeth[2†], A. Secchi[3,4‡], M. Rontani[3], D. C. Ralph[5,6], P. L. McEuen[5,6] and S. Ilani[1*]

1 Weizmann Institute of Science, Israel 2 Niels Bohr Institute, Denmark
5 Physics Department, Cornell University, Ithaca, New York

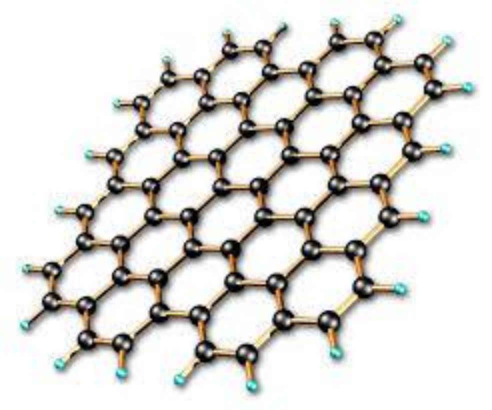
SECOND PART

Some examples of high-energy particle-physics analogies

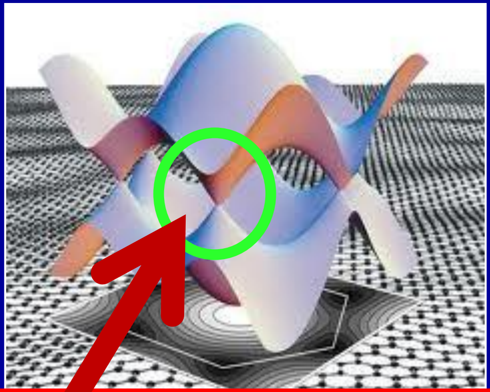
(graphene based nanosystems)

I. Romanovsky, C. Yannouleas, and U. Landman,
PRB **89,** 035432 (2014)
PRB **87,** 165431 (2013)

c → v_F



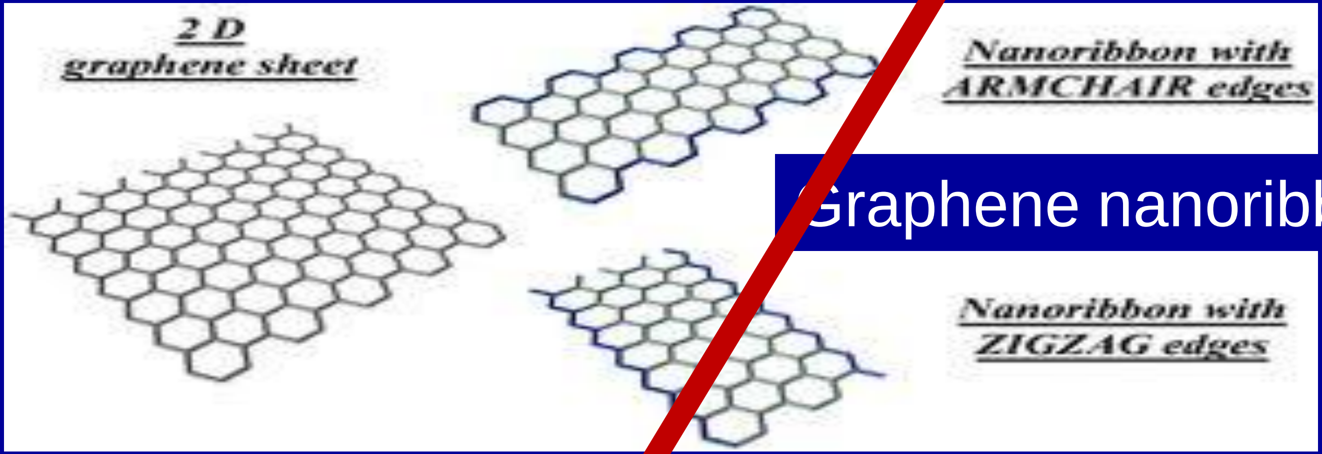
2D Graphene:
honeycomb lattice



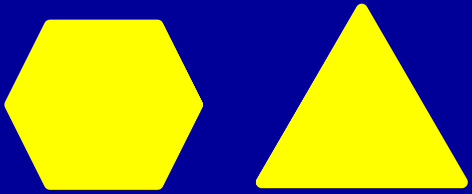
Massless Dirac-Weyl fermion

Graphene Nanosystems

Armchair or Zigzag edge terminations



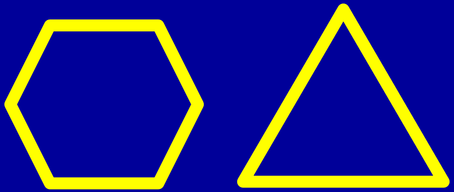
Graphene nanoribbons



Graphene quantum dots

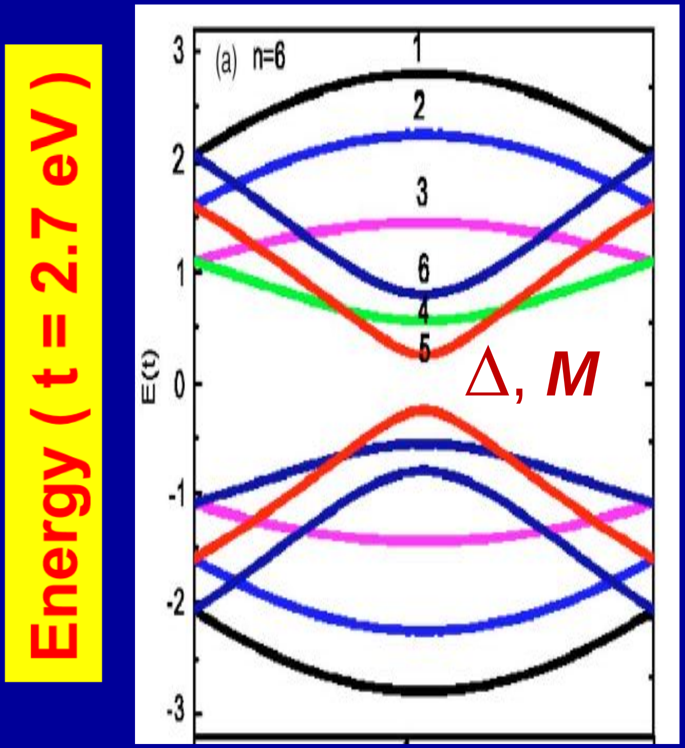
Open a gap Δ?

***M* v_F^2 = Δ**

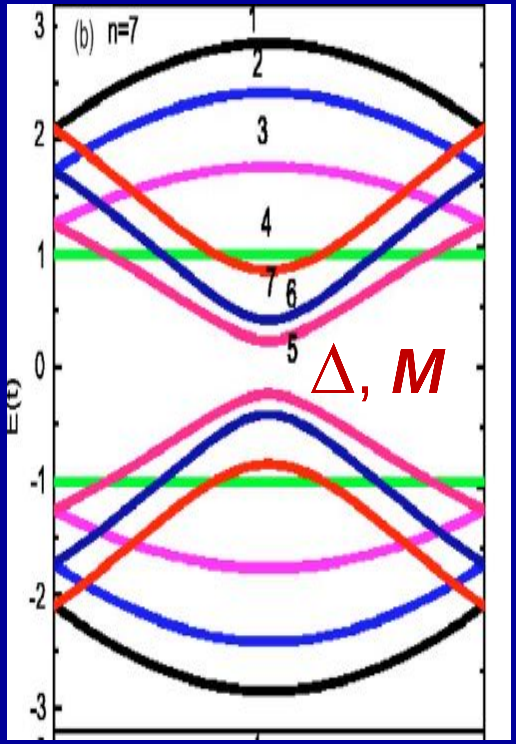


Graphene nanorings

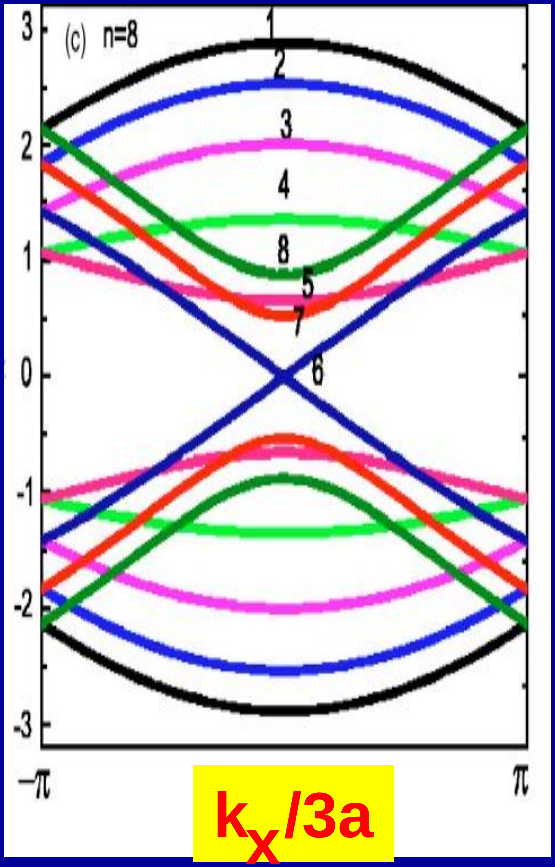
Uniform Armchair Nanoribbons



N=3m (Class I)
Semiconductor



N=3m+1 (Class II)
Semiconductor

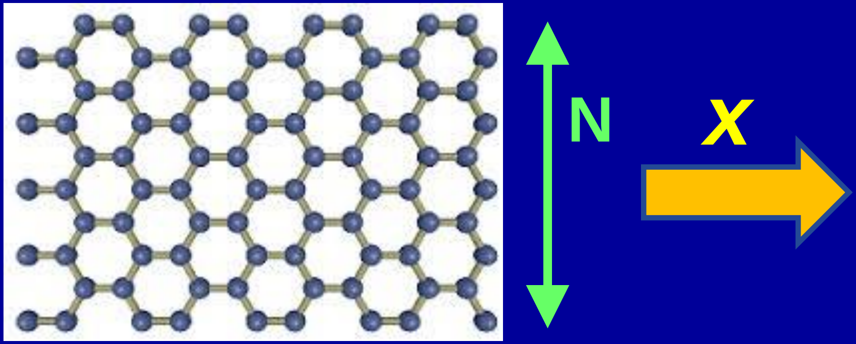


N=3m+2 (Class III)
Metallic

TB

(tight binding)

Massive Dirac

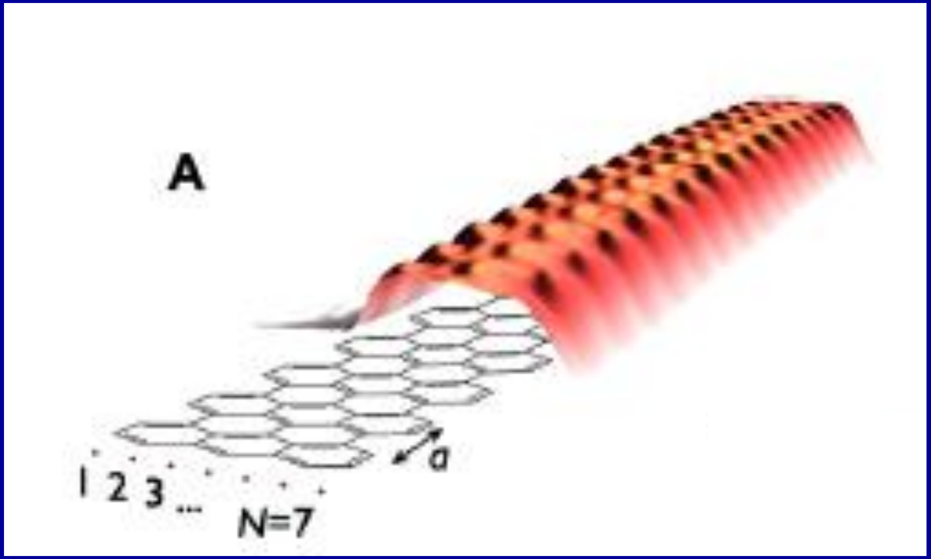


nature
Vol 466 | 22 July 2010 | doi:10.1038/nature09211

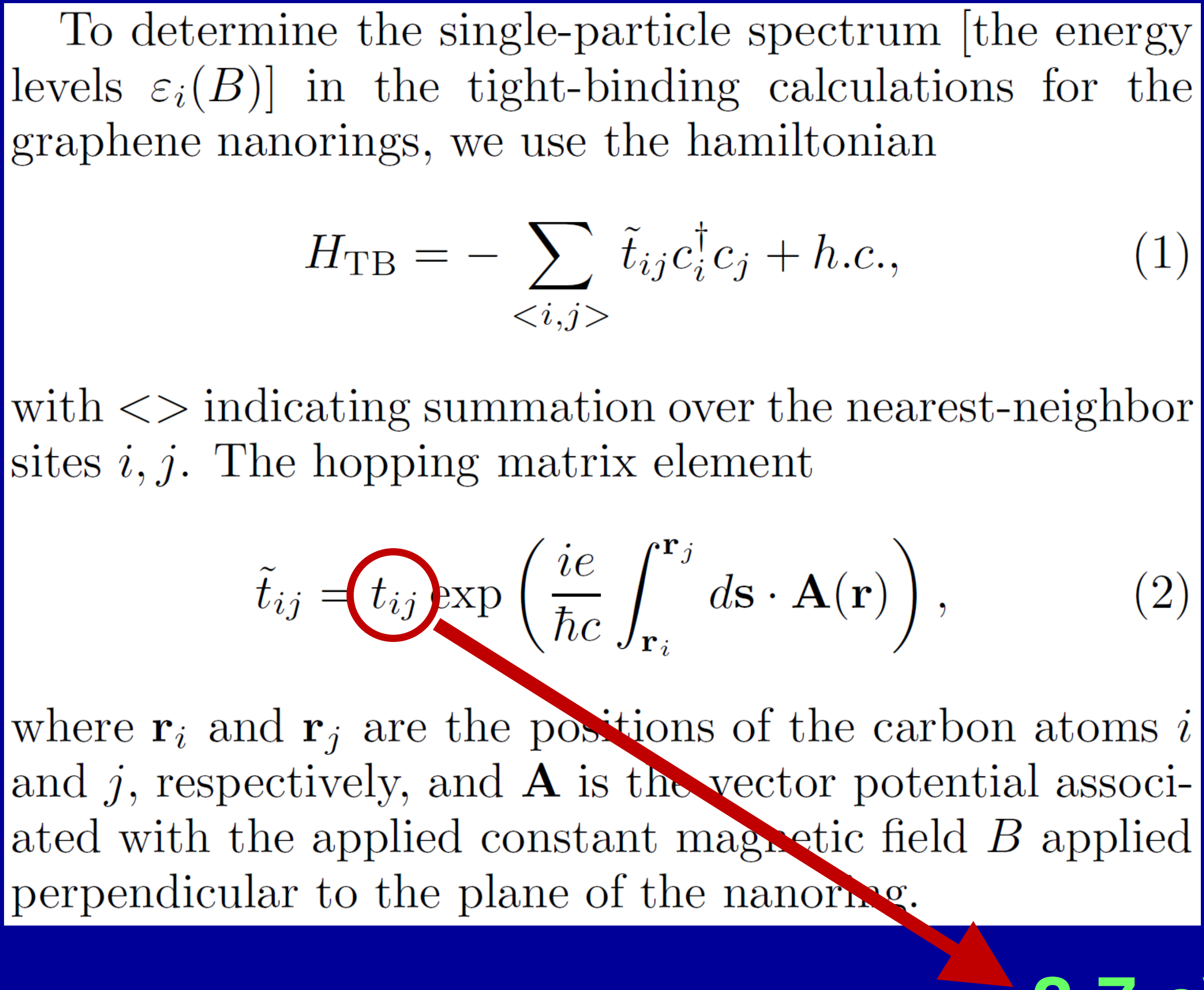
LETTERS

Atomically precise bottom-up fabrication of graphene nanoribbons

Jinming Cai[1]*, Pascal Ruffieux[1]*, Rached Jaafar[1], Marco Bieri[1], Thomas Braun[1], Stephan Blankenburg[1], Matthias Muoth[2], Ari P. Seitsonen[3,4], Moussa Saleh[5], Xinliang Feng[5], Klaus Müllen[5] & Roman Fasel[1,6]



Tight-Binding (TB)



To determine the single-particle spectrum [the energy levels $\varepsilon_i(B)$] in the tight-binding calculations for the graphene nanorings, we use the hamiltonian

$$H_{\rm TB} = - \sum_{<i,j>} \tilde{t}_{ij} c_i^\dagger c_j + h.c., \qquad (1)$$

with $<>$ indicating summation over the nearest-neighbor sites i, j. The hopping matrix element

$$\tilde{t}_{ij} = \boxed{t_{ij}} \exp\left(\frac{ie}{\hbar c} \int_{\mathbf{r}_i}^{\mathbf{r}_j} d\mathbf{s} \cdot \mathbf{A}(\mathbf{r}) \right), \qquad (2)$$

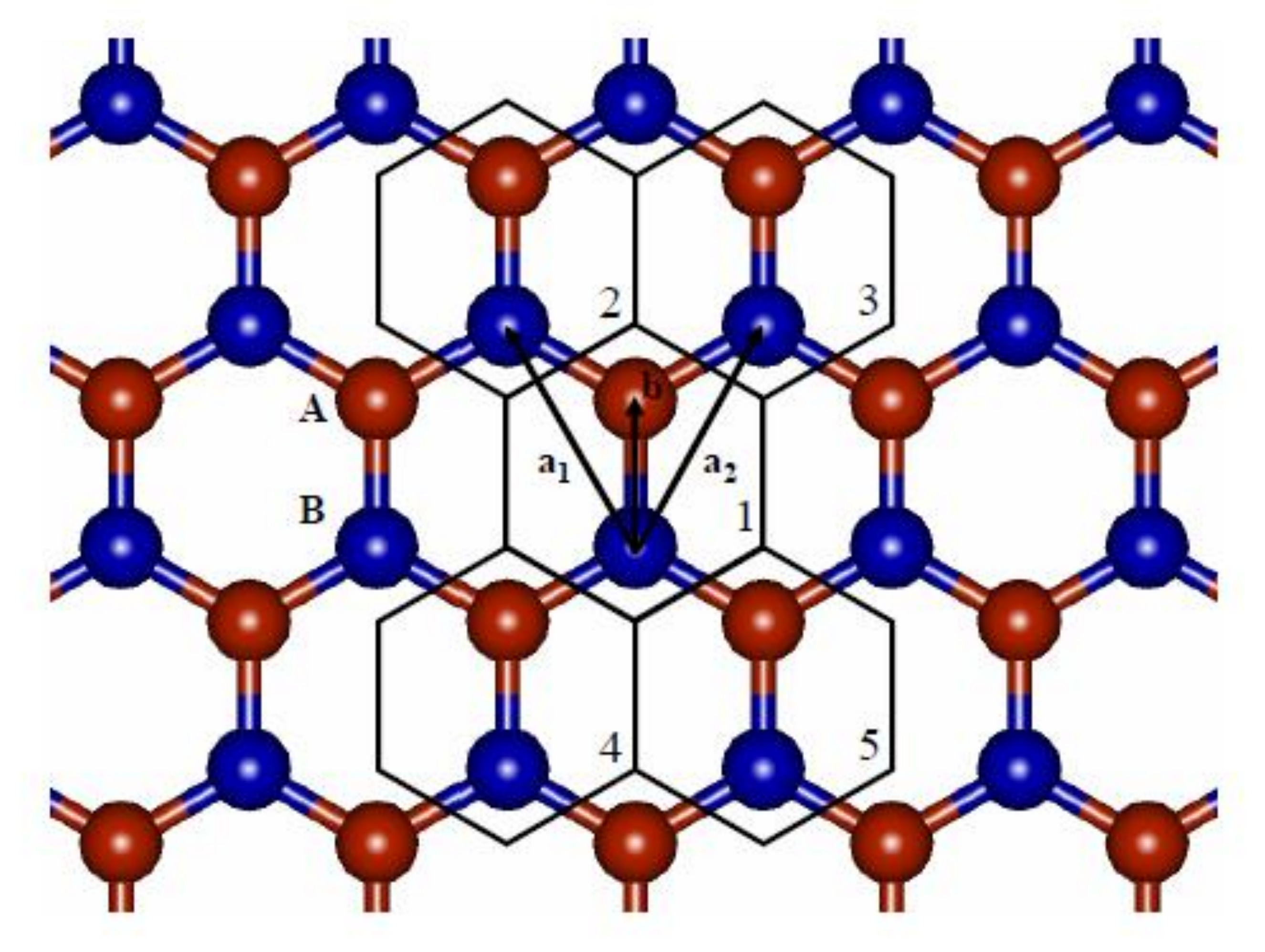
where $\mathbf{r}_i$ and $\mathbf{r}_j$ are the positions of the carbon atoms i and j, respectively, and $\mathbf{A}$ is the vector potential associated with the applied constant magnetic field B applied perpendicular to the plane of the nanoring.

2.7 eV

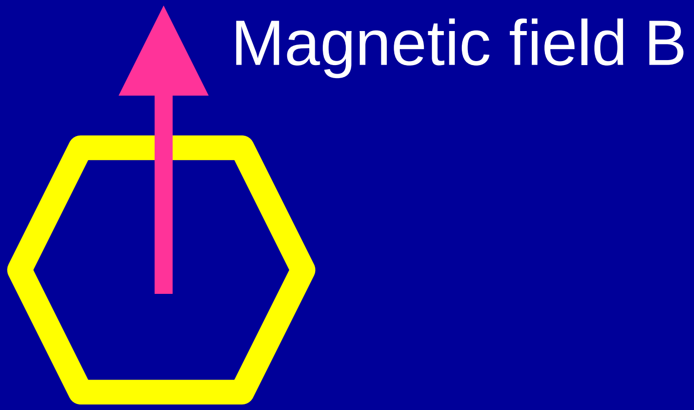
Tight-Binding (TB)

Two atoms in a unit cell/ Two sublattices

A and **B**



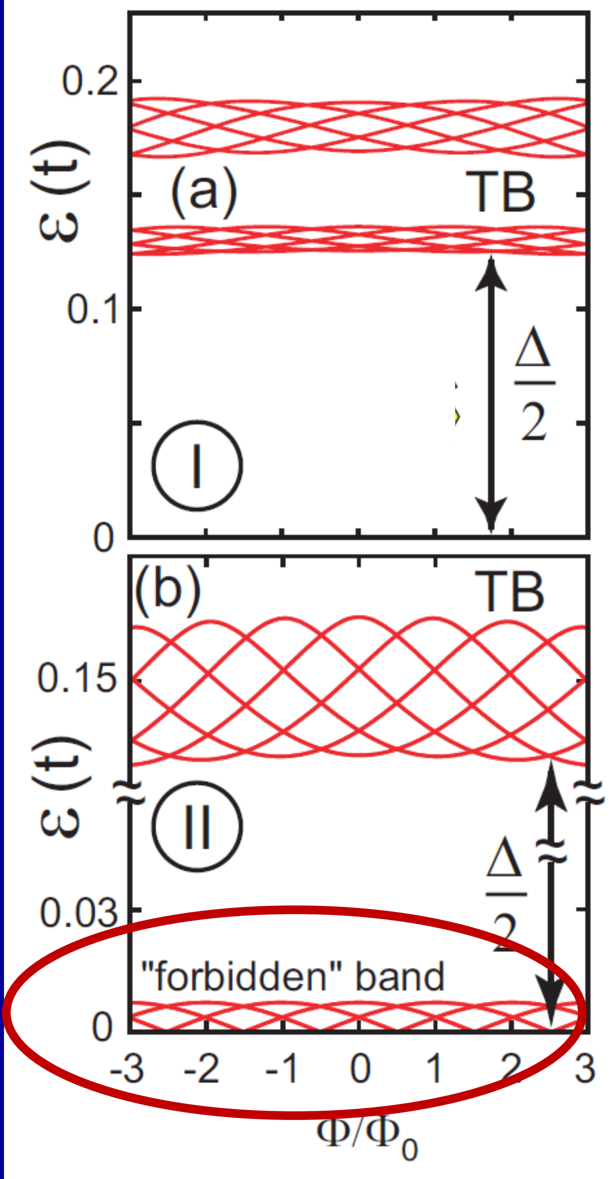
Aharonov-Bohm spectra



Hexagonal Armchair Rings with semiconducting arms

Single-particle TB spectra

N=15 (Class I)   N=16 (Class II)



Magnetic flux (magnetic field B)

1D Generalized Dirac equation

α and β: any two of the three 2x2 Pauli matrices

$$[E - V(x)]I\Psi + i\hbar v_F \alpha \frac{\partial \Psi}{\partial x} - \beta \phi(x) \Psi = 0$$

$$\Psi = \begin{pmatrix} \psi_u \\ \psi_l \end{pmatrix}$$

electrostatic potential
(Lorentz vector potential)

scalar (Higgs) field / position-dependent mass **m(x)**
(Lorentz scalar potential)

Question: Confinement of a relativistic fermion?

Problem with V(x): Klein tunneling

m(x) can confine relativistic particles

1D Generalized Dirac equation

α and **β**: any two of the three 2x2 Pauli matrices

$$[E - V(x)]I\Psi + i\hbar v_F \alpha \frac{\partial \Psi}{\partial x} - \beta\phi(x)\Psi = 0$$

$$\Psi = \begin{pmatrix} \psi_u \\ \psi_l \end{pmatrix}$$

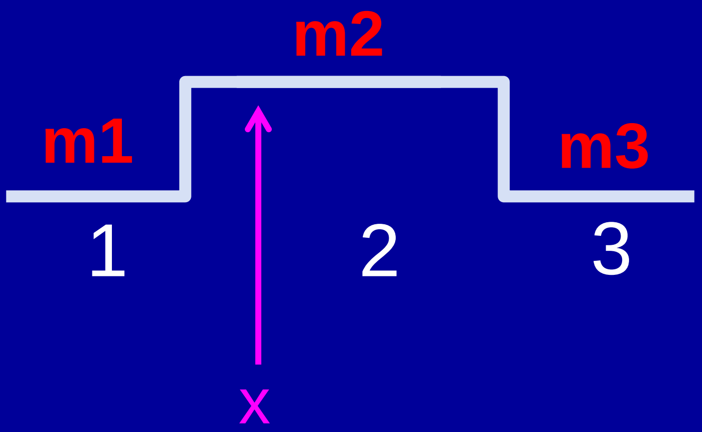
electrostatic potential

scalar (Higgs) field / position-dependent mass **m(x)**

Dirac-Kronig-Penney Superlattice

Transfer matrix method

a single side/ 3 regions



$$\boldsymbol{\Omega}_K(x) = \begin{pmatrix} e^{iKx} & e^{-iKx} \\ \Lambda e^{iKx} & -\Lambda e^{-iKx} \end{pmatrix}$$

$$K^2 = \frac{(E-V)^2 - m^2 v_F^4}{\hbar^2 v_F^2}$$

$$\Lambda = \frac{\hbar v_F K}{E - V + m v_F^2}$$

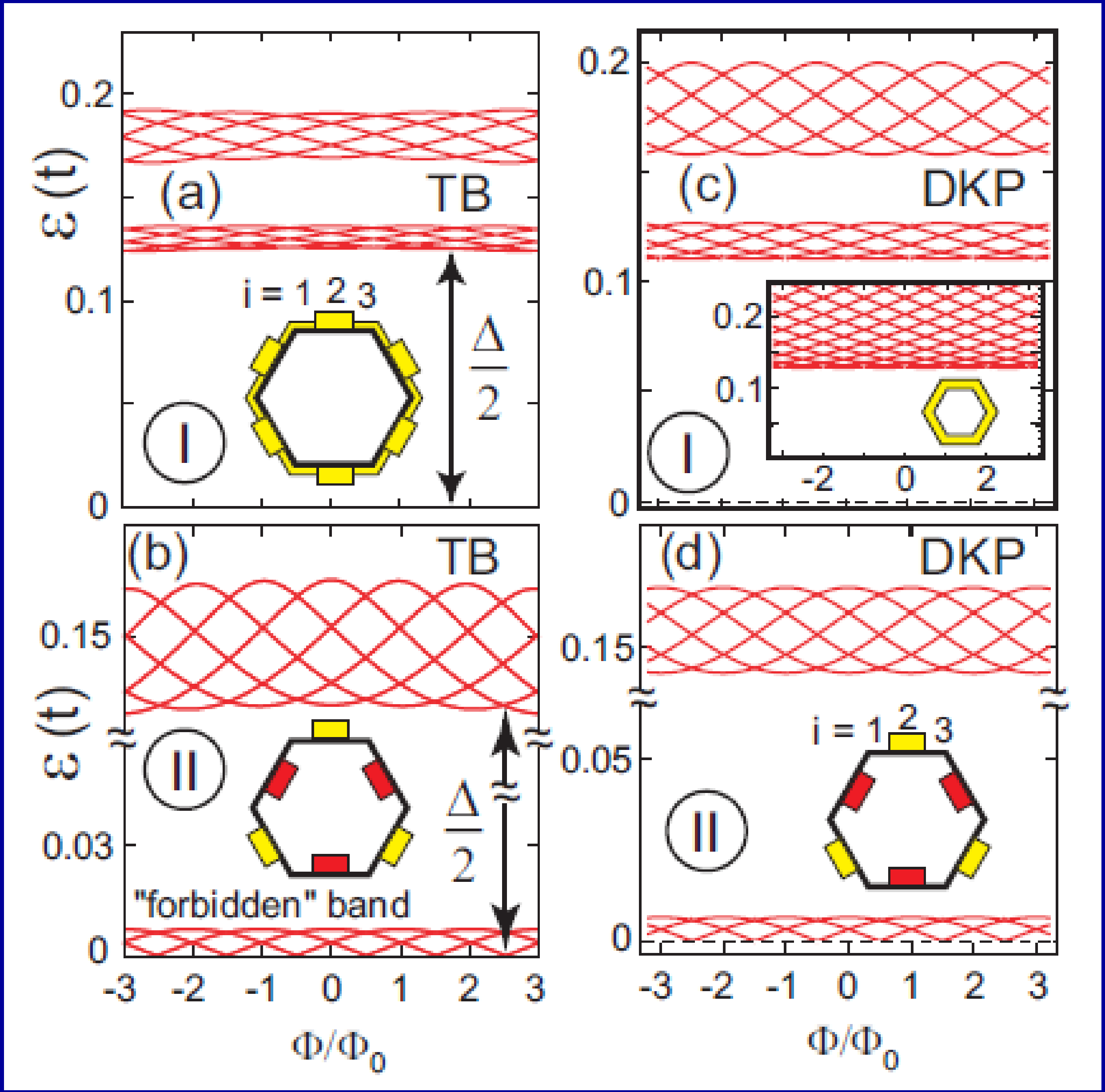
Spectra/ Armchair Rings with semi-conducting arms

Yellow: Mass > 0

Red: Mass < 0

N=15 (Class I)

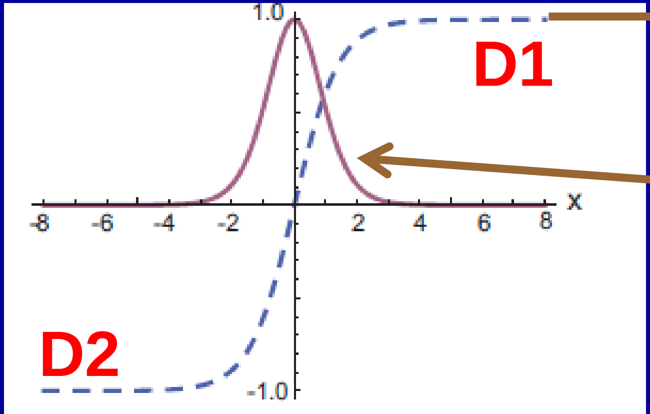
N=16 (Class II)



Magnetic flux (magnetic field B)

Jackiw-Rebbi, PRD **13**, 3398 (1976)

kink soliton/ zero-energy fermionic soliton

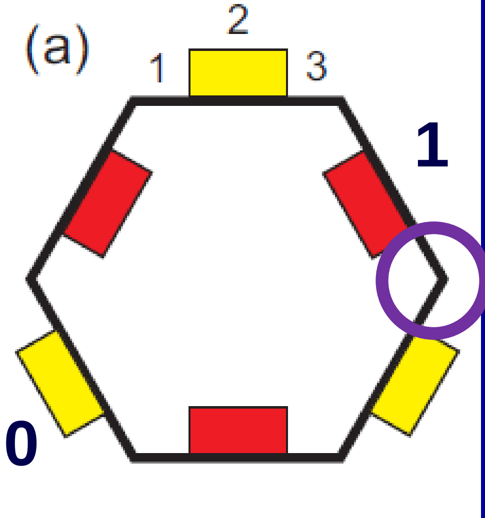


kink soliton

$$\phi_k(x) = \zeta \tanh\left(\sqrt{\frac{\xi}{2}}\zeta x\right)$$

zero-energy fermionic soliton (Dirac eq.)

$$\Psi_S(x) \propto \begin{pmatrix} \exp\left(-\int_0^x \phi_k(x')dx'\right) \\ 0 \end{pmatrix}$$

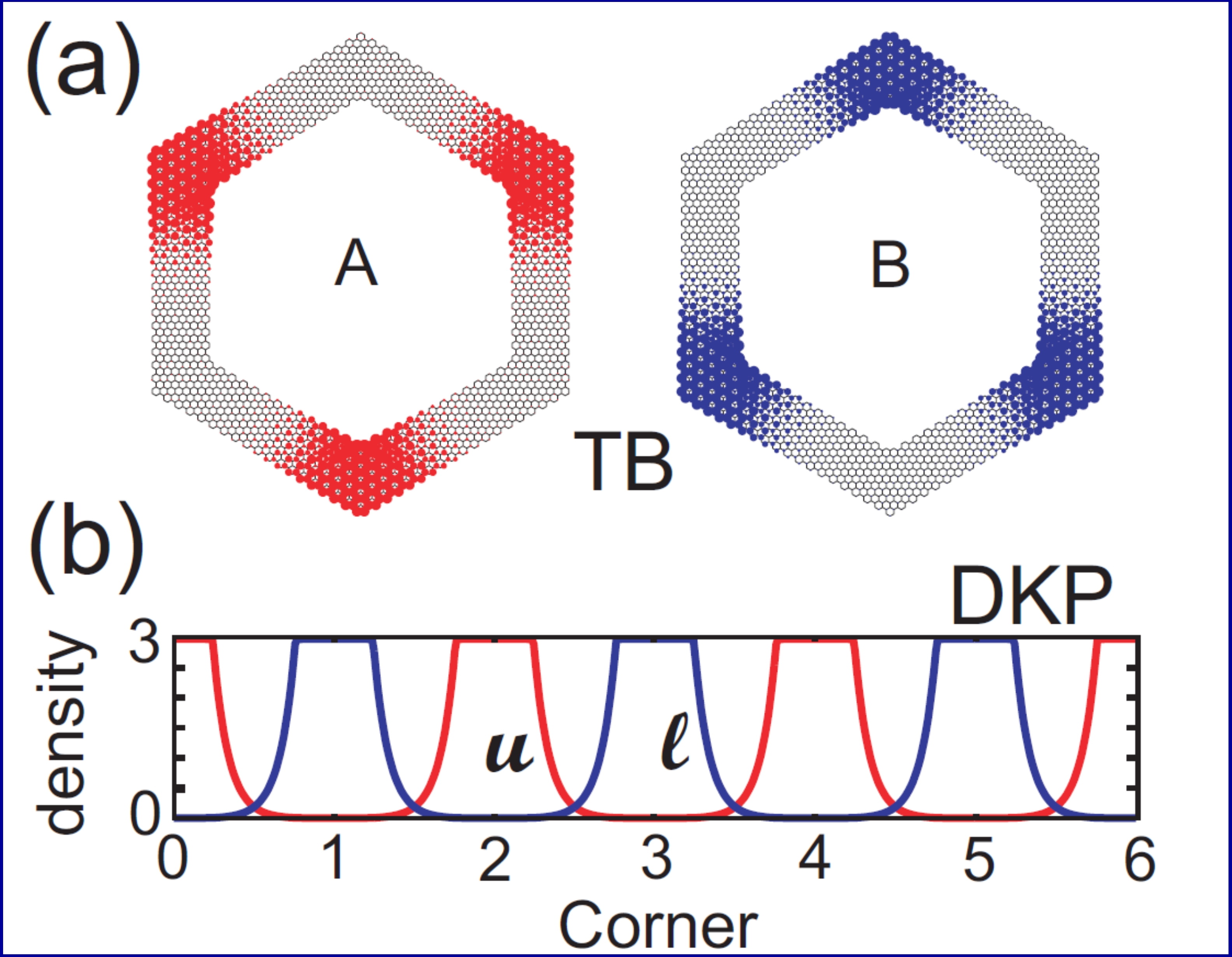


1D topological insulator

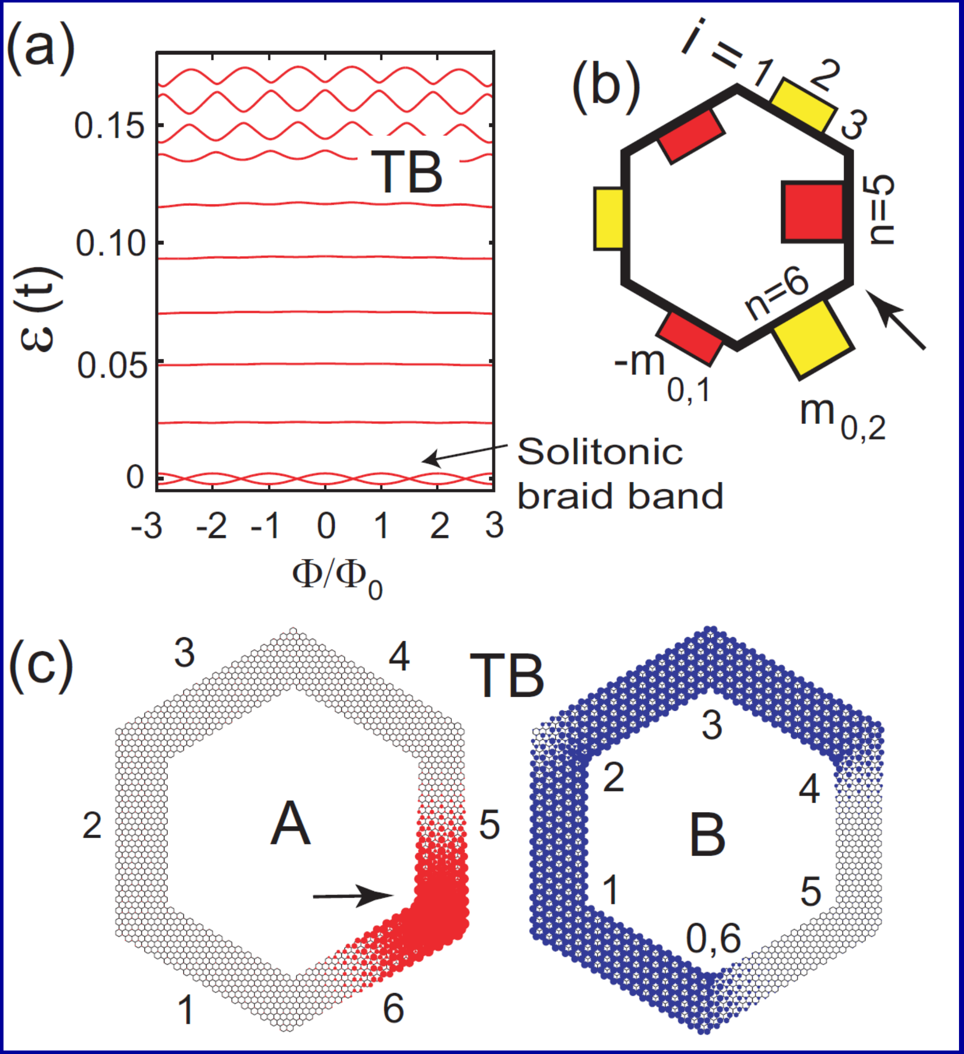
Topological invariants
(Chern numbers):
negative mass 1 (nontrivial)
positive mass 0 (trivial)

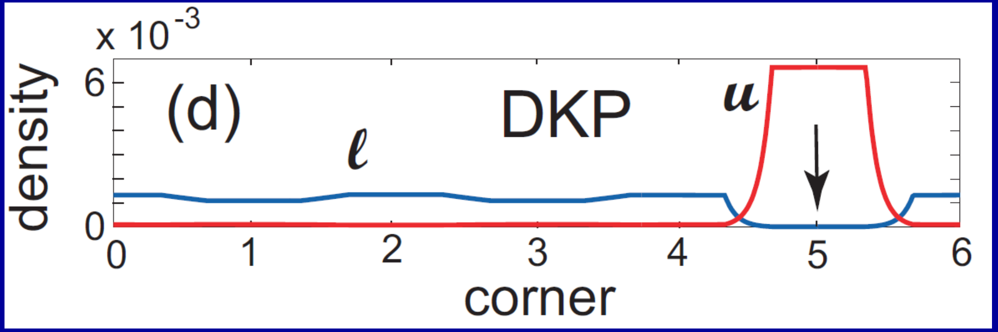
Densities for a state in the forbidden band

e/6 fractional charge



Mixed Metallic-semiconductor N=17 (Class III) / N=15 (Class I)





e/2
fractional charge

Full circle

Conclusions

1) Instead of usual quantum-size confinement effects (case of clusters/ analogies with nuclear physics) , the spectra and wave functions of quasi-1D graphene nanostructures are sensitive to the topology of the lattice configuration (edges, shape, corners) of the system .
2) The topology is captured by general, position-dependent scalar fields (variable masses, including alternating +/- masses) in the relativistic Dirac equation.
3) The topology generates rich analogies with 1D quantum-field theories, e.g., localized fermionic solitons with fractional charges associated with the Jackiw-Rebbi model [PRD 13, 3398 (1976)]
4) Semiconducting hexagonal rings behave as 1D topological insulators with states well isolated from the environment (zero-energy states within the gap with charge accumulation at the corners).