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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
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 quasi-parabolic confinement potential. Sweeping the plunger-gate voltage tunes both the shape and the chemical potential of the quantum dot.

**Lateral QD (Ottawa)**

**Vertical QD (Delft)**

**Electrostatic confinement**

**Lateral QD Molecule (Delft)**
CONTROL PARAMETERS FOR SYMMETRY BREAKING

IN SINGLE QD'S: WIGNER CRYSTALLIZATION

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

$$R_W = \left( \frac{e^2}{\kappa I_0} \right)/\hbar\omega_0 \sim 1/\left( \hbar^3 \omega_0 \right)^{1/2}$$

- e-e Coulomb repulsion
- kinetic energy

$$I_0 = \left( \frac{\hbar}{m^*\omega_0} \right)^{1/2}$$

Spatial Extent of 1s s.p. state

$\kappa$: dielectric const. (12.9)

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

$\hbar\omega_0 (5 - 1 \text{ meV}) \Rightarrow R_W (1.48 - 3.31)$

- 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 ($B$)

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

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

Y&L, PRL 82, 5325 (1999)

Restoration of symmetry ➔ Quantum crystal

Circular external confinement

\[ B = 0 \]

\[ R_W = 5 \]

Concentric rings: (1,6,12)

Rotating Boson Molecules (Circular trap)
Ground states: Energy, angular momentum and probability densities.

\[ R_\delta = 50 \quad R_W = 10 \]

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

\[
\rho(r | r_0) = \langle \Phi | \sum_{i \neq j} \delta(r_i - r)\delta(r_j - r_0) | \Phi \rangle / \langle \Phi | \Phi \rangle
\]
Three electron anisotropic QD

Method: Exact Diagonalization (EXD)

Electron Density (ED)

Conditional Probability Distribution (CPD)


Anisotropic confinement

EXD wf $\sim |\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\uparrow\rangle$

Entangled three-qubit W-states
### WAVE-FUNCTION BASED APPROACHES

#### TWO-STEP METHOD

**A HIERARCHY OF APPROXIMATIONS**

<table>
<thead>
<tr>
<th>Total Energy</th>
<th>Correlations</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Restricted Hartree-Fock (RHF)</strong></td>
<td><strong>Non-linear equations</strong></td>
</tr>
<tr>
<td>All spin and space symmetries are preserved</td>
<td></td>
</tr>
<tr>
<td>Double occupancy / e-densities: circularly symmetric</td>
<td><strong>EMERGENT PHENOMENA</strong></td>
</tr>
<tr>
<td><strong>Single Slater determinant (central mean field)</strong></td>
<td></td>
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<tr>
<td><strong>Unrestricted Hartree-Fock (UHF)</strong></td>
<td>Restoration of linearity of many-body equations</td>
</tr>
<tr>
<td>Total-spin and space symmetries (rotational or parity) are broken / Different orbitals for different spins</td>
<td></td>
</tr>
<tr>
<td>Solutions with lower symmetry (point-group symmetry)</td>
<td></td>
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<tr>
<td>Lower symmetry explicit in electron densities</td>
<td></td>
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<tr>
<td><strong>Single Slater determinant (non-central mean field)</strong></td>
<td></td>
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<tr>
<td>Implementation of UHF: Pople-Nesbet Eqs.</td>
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<tr>
<td>2D harmonic-oscillator basis set</td>
<td></td>
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<tr>
<td>Two coupled matrix Eqs. (for up and down spins)</td>
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<tr>
<td>Restoration of symmetry via projection techniques</td>
<td></td>
</tr>
<tr>
<td><strong>Superposition of UHF Slater det.’s (beyond mean field)</strong></td>
<td></td>
</tr>
<tr>
<td>e-densities: circularly symmetric</td>
<td></td>
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<tr>
<td>Good total spin and angular momenta</td>
<td></td>
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<tr>
<td>Lower symmetry is INTRINSIC (or HIDDEN)</td>
<td></td>
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<tr>
<td>Detection of broken symmetry: CPDs and rovibrational excitations of quantum dots</td>
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<tr>
<td>CPDs and dissociation of quantum dot molecules</td>
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</tbody>
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**EXACT DIAGONALIZATION**

*(Full Configuration Interaction)*

When possible *(small N): High numerical accuracy*

**Physics less transparent compared to “THE TWO-STEP”**

Pair correlation functions, **CPDs**

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*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

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. Gossard3
1 Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland
2 School of Physics, Georgia Institute 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.

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

S. Pecker1†, F. Kuemmeth2†, A. Secchi3,4‡, M. Rontani3, D. C. Ralph5,6, P. L. McEuen5,6 and S. Ilani1*
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)
2D Graphene: honeycomb lattice

Graphene Nanosystems

Armchair or Zigzag edge terminations

Graphene quantum dots

Graphene nanoribbons

Open a gap $\Delta$?

$M v_F^2 = \Delta$
Uniform Armchair Nanoribbons

$N=3m$ (Class I) Semiconductor

$N=3m+1$ (Class II) Semiconductor

$N=3m+2$ (Class III) Metallic

$\Delta, M$

$\frac{k_x}{3a}$

TB (tight binding)
LETTERS

Atomically precise bottom-up fabrication of graphene nanoribbons

Jinming Cai¹, Pascal Ruffieux¹*, Rached Jaafar¹, Marco Bieri¹, Thomas Braun¹, Stephan Blankenburg¹, Matthias Muoth², Ari P. Seitsonen³,⁴, Moussa Saleh⁵, Xinliang Feng⁵, Klaus Müller⁵ & Roman Fasel¹,⁶
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

$$H_{\text{TB}} = - \sum_{\langle i,j \rangle} \tilde{t}_{ij} c_i^\dagger c_j + h.c., \quad (1)$$

with $\langle \rangle$ indicating summation over the nearest-neighbor sites $i, j$. The hopping matrix element

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

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.
Two atoms in a unit cell/
Two sublattices A and B

Tight-Binding (TB)
Hexagonal Armchair Rings with semiconducting arms

Single-particle TB spectra

Magnetic field $B$

N=15 (Class I)

N=16 (Class II)

Aharonov-Bohm spectra

Magnetic flux (magnetic field $B$)
1D Generalized Dirac equation

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

\[ \Psi = \begin{pmatrix} \psi_u \\ \psi_i \end{pmatrix} \]

\( \alpha \) and \( \beta \): any two of the three 2x2 Pauli matrices

- 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
The 1D Generalized Dirac equation is given by:

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

where \( \alpha \) and \( \beta \) are any two of the three 2x2 Pauli matrices. The solution is expressed as:

\[
\Psi = \begin{pmatrix} \psi_u \\ \psi_l \end{pmatrix}
\]

The electrostatic potential \( \phi(x) \) and scalar (Higgs) field / position-dependent mass \( m(x) \) are considered.

The Dirac-Kronig-Penney Superlattice consists of a single side with 3 regions:

- Region 1: Mass \( m_1 \)
- Region 2: Mass \( m_2 \)
- Region 3: Mass \( m_3 \)

The transfer matrix is:

\[
\Omega_K(x) = \begin{pmatrix} e^{iKx} & e^{-iKx} \\ \Lambda e^{iKx} & -\Lambda e^{-iKx} \end{pmatrix}
\]

The wave number \( K \) is given by:

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

And the phase factor \( \Lambda \) is:

\[
\Lambda = \frac{\hbar v_F K}{E - V + mv_F^2}
\]
Spectra/Armchair Rings with semi-conducting arms

Yellow:
Mass > 0

Red:
Mass < 0

Magnetic flux (magnetic field B)
kink soliton/ zero-energy fermionic soliton

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

zero-energy fermionic soliton (Dirac eq.)

\[ \Psi_S(x) \propto \left( \exp \left( - \int_0^x \phi_k(x')dx' \right) \right) \]

1D topological insulator

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

Jackiw-Rebbi, PRD 13, 3398 (1976)
Densities for a state in the forbidden band

\[ \frac{e}{6} \] fractional charge

(a)

(b)

Corner

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

e/2 fractional charge
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).