NUCLEAR AND PARTICLE-PHYSICS ASPECTS OF CONDENSED-MATTER NANOSYSTEMS

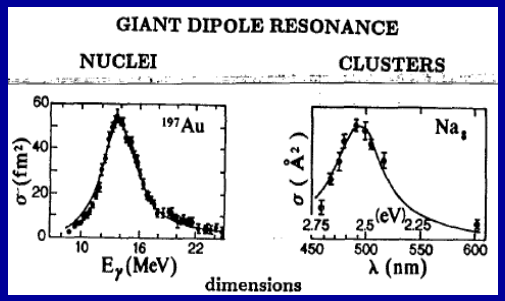
Constantine Yannouleas and Uzi Landman
School of Physics, Georgia Institute of Technology

Common challenges in finite fermion systems, Buffalo, NY, 6-8 November 2013

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

Three (among others) major nuclear aspects:

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



- *Electronic shells/deformation/fission*
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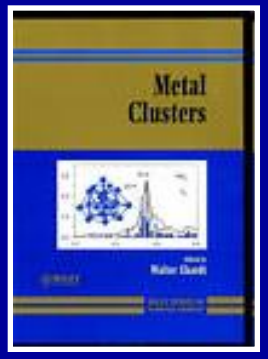
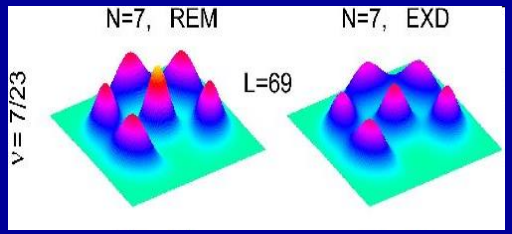


- *Strongly correlated states (Quantum crystals/Wigner molecules/dissociation)*
  in 2D semiconductor quantum dots and
  ultracold bosonic traps via
  symmetry breaking/symmetry restoration
  in conjunction with exact diagonalization (full CI)
  [see, e.g., Yannouleas, Landman,
  Rep. Prog. Phys. **70,**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



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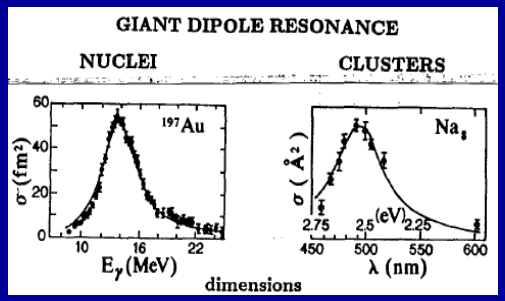

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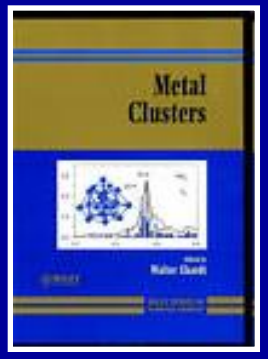


- *Strongly co...*
  in 2D semi...
  ultracold bo...
  symmetry b...
  in conjunct...
  [see, e.g., Ya...
  Rep. Prog. Ph...

KS-DFT

NO KS-DFT/ due to the self-interaction error, and to the open problem of how to use multi-determinants and to restore symmetries in DFT

TWO VARIANTS OF SHELL CORRECTION METHOD (SCM) in condensed-matter nanosystems:

1) Fully microscopic (DFT-SCM) / **Orbital-free DFT**

Based on Extended Thomas Fermi (ETF)
sp densities and central potentials

Literature: **Y&L,** PRB **48**, 8376 (1993) (multiply anionic metal clusters)

Y&L, Ch. 7 in "Recent Advances in Orbital-Free Density Functional Theory," Y.A. Wang and T.A. Wesolowski Eds. (Word Scientific, Singapore, 2013)
(metal clusters, nanowires, fullerenes)

2) Semiempirical (SE-SCM)

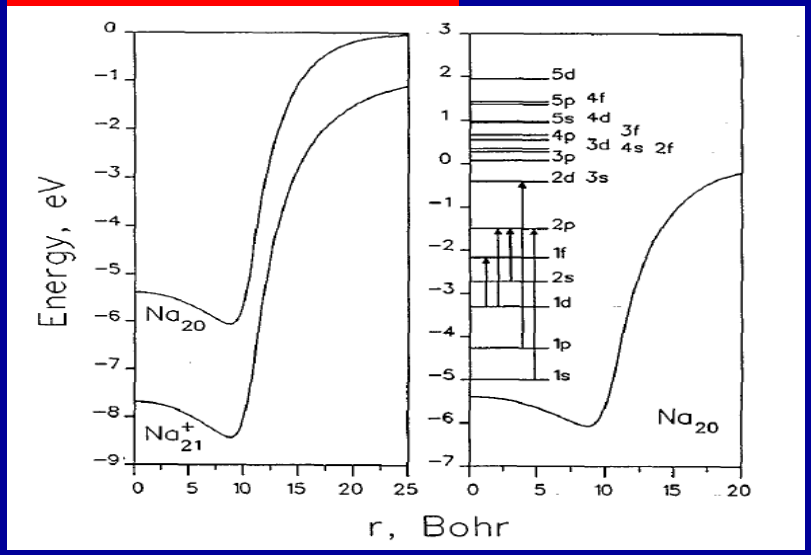
Based on a triaxial H.O. (Nilsson) central potential
+ liquid drop model for smooth variation

Y&L, PRB **51**, 1902 (1995) (deformed metal clusters)

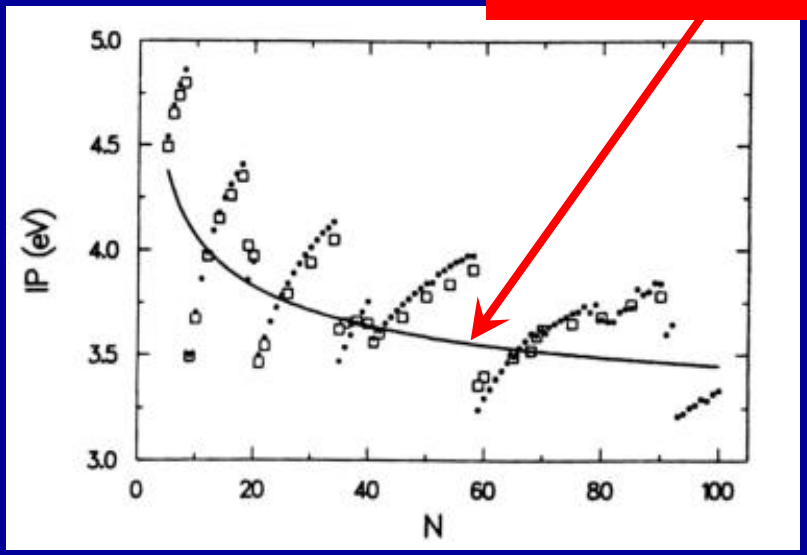
Used extensively in nuclear physics

SCM-DFT (based on ETF) ➡ KS-DFT

ETF potentials



ETF/ Smooth



Yannouleas & Landman,
PRB **48**, 8376 (1993)

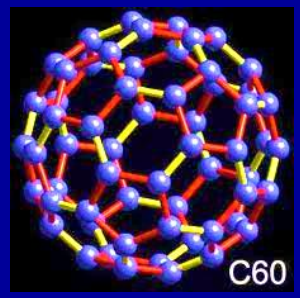
$$T_{sh} = \sum_{i=1}^{\text{occ}} \widetilde{\varepsilon}_i - \int \rho_{ETF}(\mathbf{r}) V_{ETF}(\mathbf{r}) d\mathbf{r},$$

Shell correction: Difference of two kinetic energy terms

$$\Delta E_{sh} = T_{sh} - T_{ETF}[\rho_{ETF}]$$

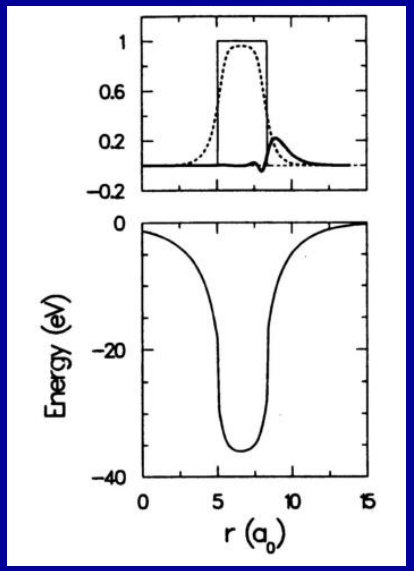
Applications of DFT-SCM: neutral fullerene C_{60}

Y&L, Chem. Phys. Lett. **217**, 175 (1994)



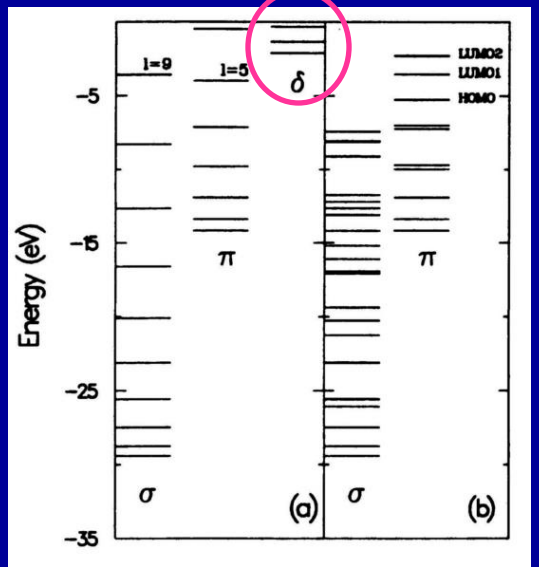
ETF density

ETF potential



Spherical

Icosahedral

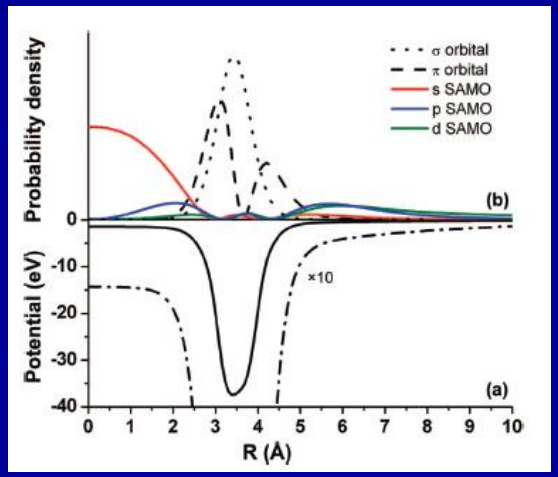


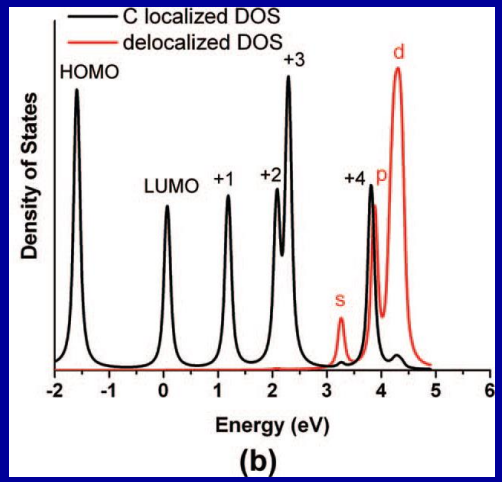
The Superatom States of Fullerenes and Their Hybridization into the Nearly Free Electron Bands of Fullerites

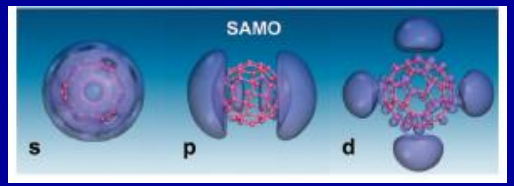
J. Zhao, M. Feng, J. Yang, H. Petek

ACS Nano **3**, 854 (2009)

LT-STM







SECOND PART

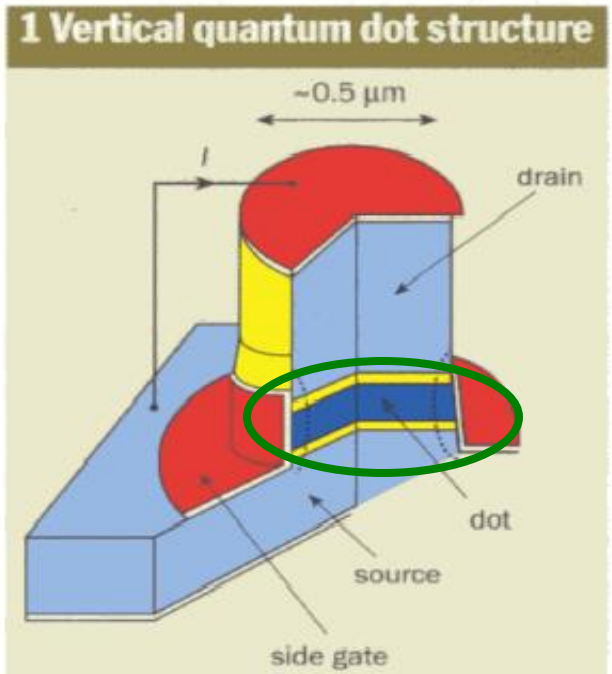
Strong correlations and symmetry breaking/restoration in 2D finite systems

Constantine Yannouleas and Uzi Landman

Phys. Rev. Lett. **82**, 5325 (1999);
Rep. Prog. Phys. **70**, 2067 (2007)

Collaborators:

Igor Romanovsky (ultracold bosons & graphene nanostructures)
Yuesong Li (electrons in QDs)
Ying Li (electrons in Quantum Dot Molecules)
Leslie O. Baksmaty (ultracold bosons & electrons in QDs)



Vertical QD (Delft)

Electrostatic confinement

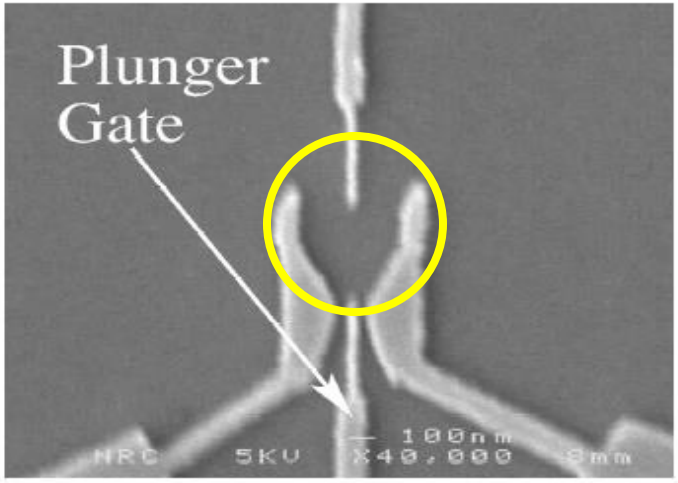
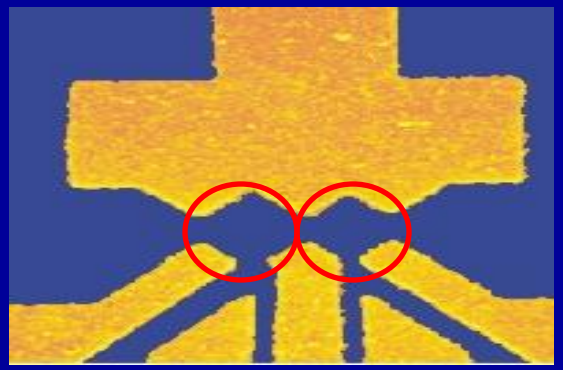


FIG. 1. SEM image of the gate geometry forming the quantum dot. This geometry enables a precisely known number of electrons ($N = 0,1,2,\ldots,50$) to be trapped (Ref. 13) and produces a quasiparabolic confinement potential. Sweeping the plunger-gate voltage tunes both the shape and the chemical potential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

Lateral QD (Ottawa)

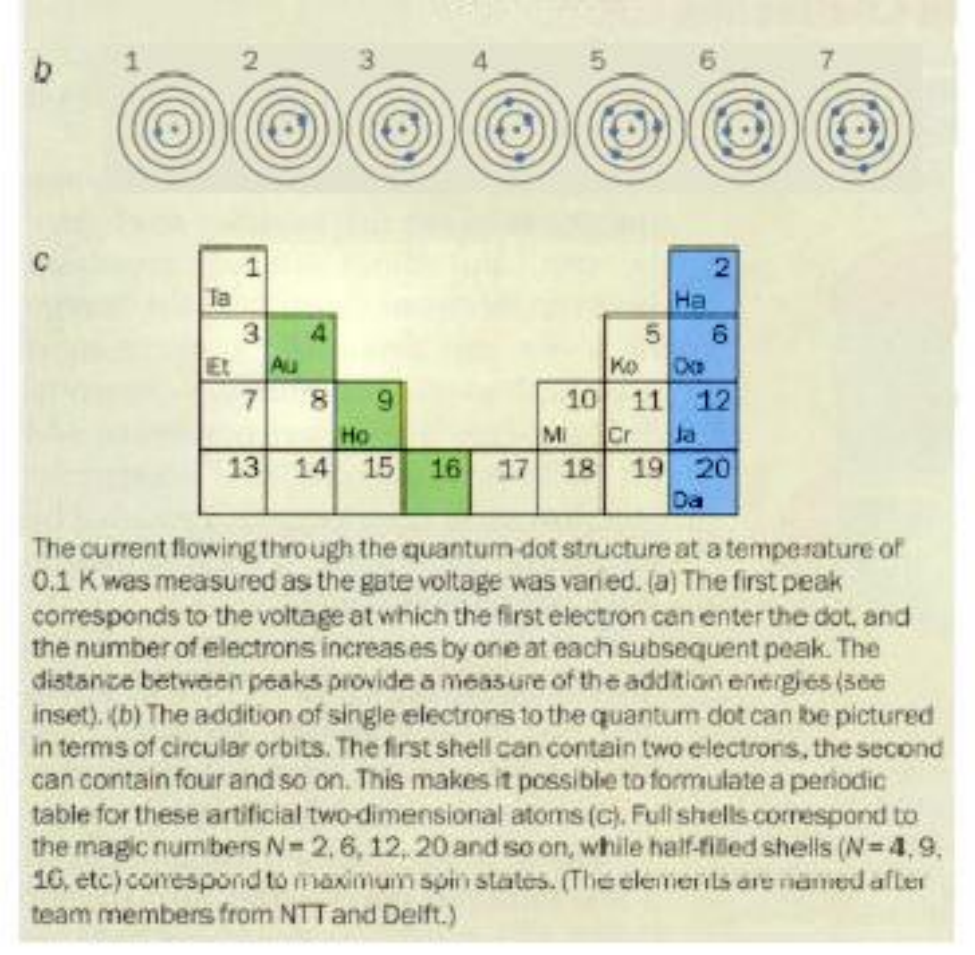


Lateral QD Molecule (Delft)

Central common confining potential?
Electronic Shells? (B=0; Circular QD)

2D Periodic Table?

4, 9, 16
Hund's Rule



The current flowing through the quantum-dot structure at a temperature of 0.1 K was measured as the gate voltage was varied. (a) The first peak corresponds to the voltage at which the first electron can enter the dot, and the number of electrons increases by one at each subsequent peak. The distance between peaks provide a measure of the addition energies (see inset). (b) The addition of single electrons to the quantum dot can be pictured in terms of circular orbits. The first shell can contain two electrons, the second can contain four and so on. This makes it possible to formulate a periodic table for these artificial two-dimensional atoms (c). Full shells correspond to the magic numbers $N = 2, 6, 12, 20$ and so on, while half-filled shells ($N = 4, 9, 16$, etc) correspond to maximum spin states. (The elements are named after team members from NTT and Delft.)

2, 6, 12, 20

Closed Shells

Kouwenhoven and Marcus, Physics World, June 1998

Wigner Crystals

DECEMBER 1, 1934 PHYSICAL REVIEW VOLUME 46

On the Interaction of Electrons in Metals

E. WIGNER, *Princeton University*

(Received October 15, 1934)

The energy of interaction between free electrons in an electron gas is considered. The interaction energy of electrons with parallel spin is known to be that of the space charges plus the exchange integrals, and these terms modify the shape of the wave functions but slightly. The interaction of the electrons with antiparallel spin, contains, fact that the electrons repell each other and try to keep as far apart as possible. The total energy of the system will be decreased through the corresponding modification of the wave function. In the present paper it is attempted to calculate this "correlation energy" by an approximation method which is, essentially, a development of the energy

… electrons repell each other and try to keep as far apart as possible. The total energy of the system will be decreased through the corresponding modification of the wave function.

… "correlation energy" …

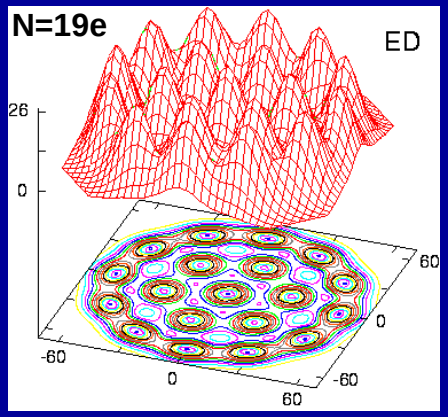
"If the electrons had no kinetic energy, they settle in configurations which correspond to the absolute minima of the potential energy. These are close-packed lattice configurations, with energies very near to that of the body-centered lattice … "

WC: Classical Electron Crystals/ Mean Field/ Broken Symmetry

Our work: Quantum Crystals/ Beyond Mean Field/ Full Symmetry

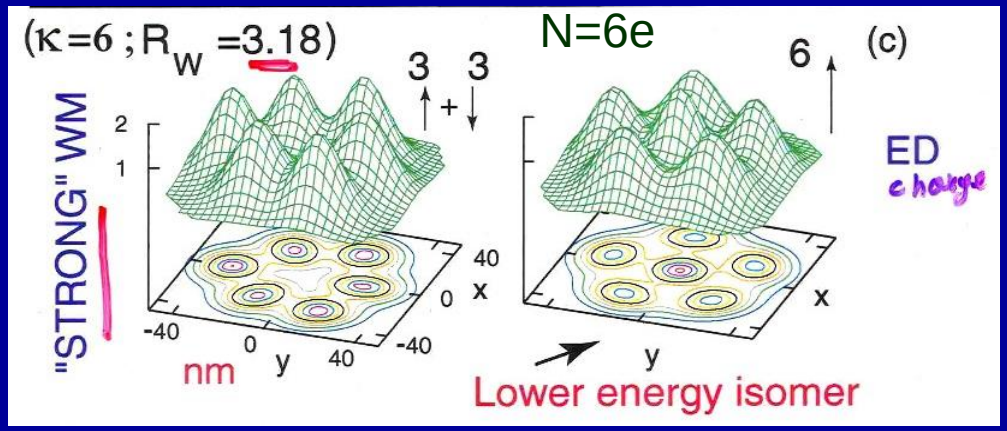
Circular external confinement

Wigner molecule in a 2D circular QD.
Electron density (ED) from
Unrestricted Hartree-Fock (UHF).
Symmetry breaking (localized orbitals).
Concentric polygonal rings



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

HAMILTONIAN FOR CLEAN 2D QD'S AND QDM'S

$$\mathcal{H} = \sum_{i=1}^{N_e} H(i) + \sum_{i=1}^{N_e} \sum_{j>i} \frac{e^2}{\kappa r_{ij}}$$

$$H(i) = H_0(i) + H_B(i)$$

$$\frac{\vec{p}_i^{\,2}}{2m^*} + V(x_i, y_i)$$

External confinement

Parabolic, single QD

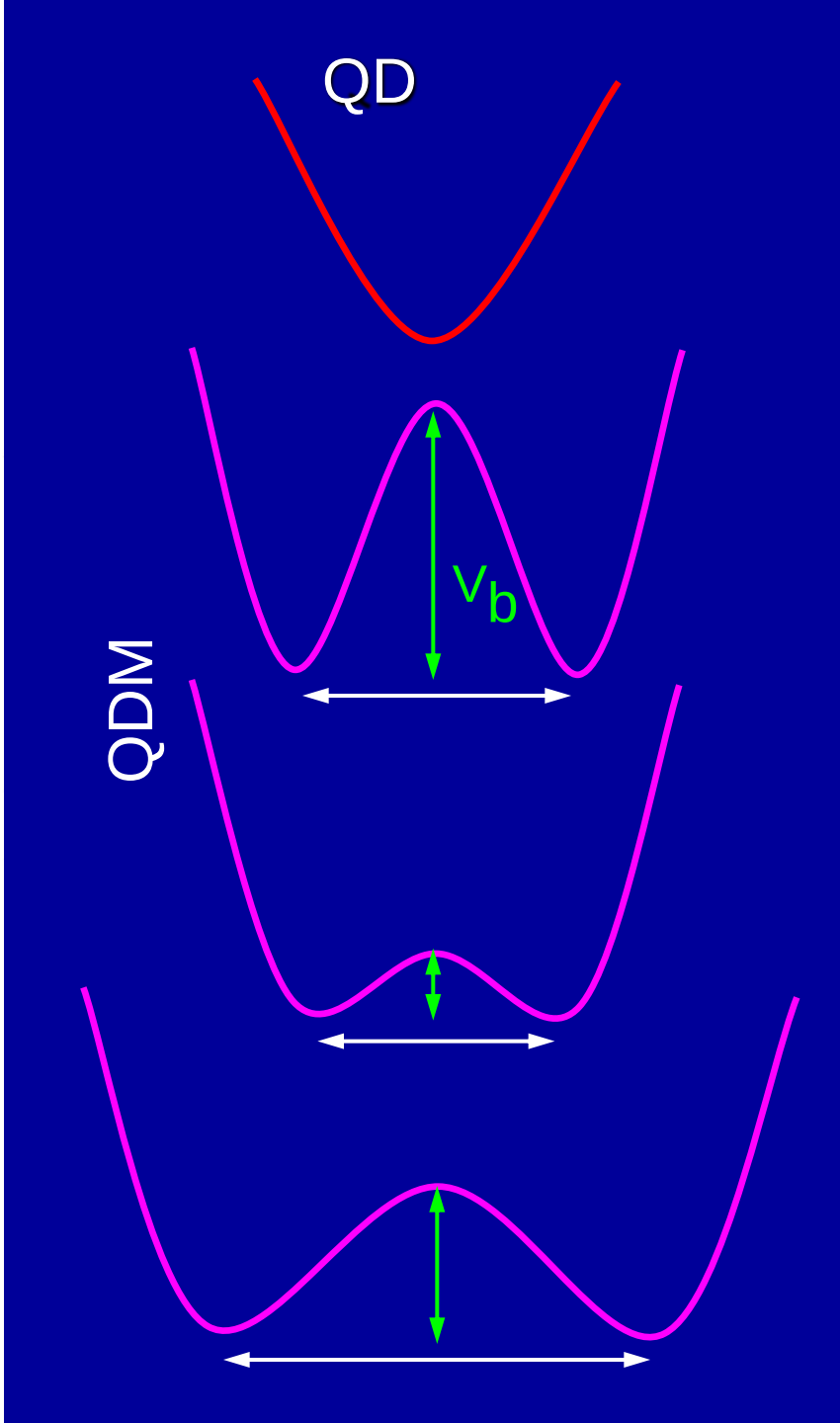
Two-center oscillator with V_b control } QDM

$$[(\vec{p}_i - e\vec{A}_i/c)^2 - \vec{p}_i^{\,2}]/2m^* + g^* \mu_B \vec{B}\cdot\vec{S}_i/\hbar$$

$$\vec{A}_i = B\,(-y_i, x_i, 0)/2$$

Zeeman

$\mathcal{H}$ can be generalized to:
Multi-component systems



HAMILTONIAN FOR CLEAN 2D QD'S AND QDM'S

$$\mathcal{H} = \sum_{i=1}^{N_e} H(i) + \sum_{i=1}^{N_e} \sum_{j>i} g\,\delta(\mathbf{r}_i - \mathbf{r}_j)$$

$$H(i) = H_0(i) + H_B(i)$$

$$\frac{\vec{p}_i^{\,2}}{2m^*} + V(x_i, y_i)$$

External confinement

Parabolic, single QD

Two-center oscillator with V_b control } QDM

Ω

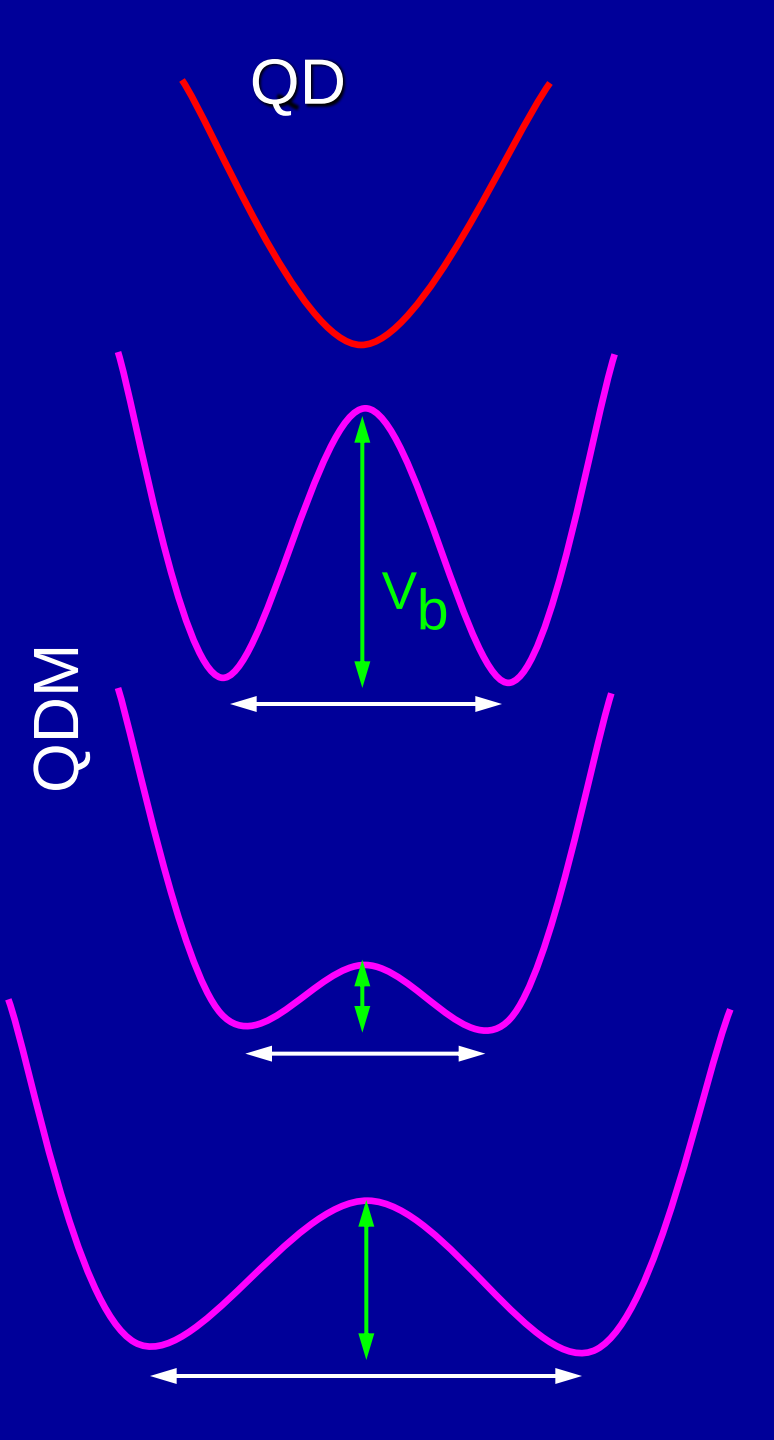
$$[(\vec{p}_i - e\vec{A}_i/c)^2 - \vec{p}_i^{\,2}]/2m^* + g^* \mu_B \vec{B}\cdot\vec{S}_i/\hbar$$

$$\vec{A}_i = B\,(-y_i, x_i, 0)/2$$

Zeeman

$\mathcal{H}$ can be generalized to Multi-component syste

Neutral Bosonic systems



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

$$l_0 = (\hbar/m^*\omega_0)^{1/2}$$ } 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

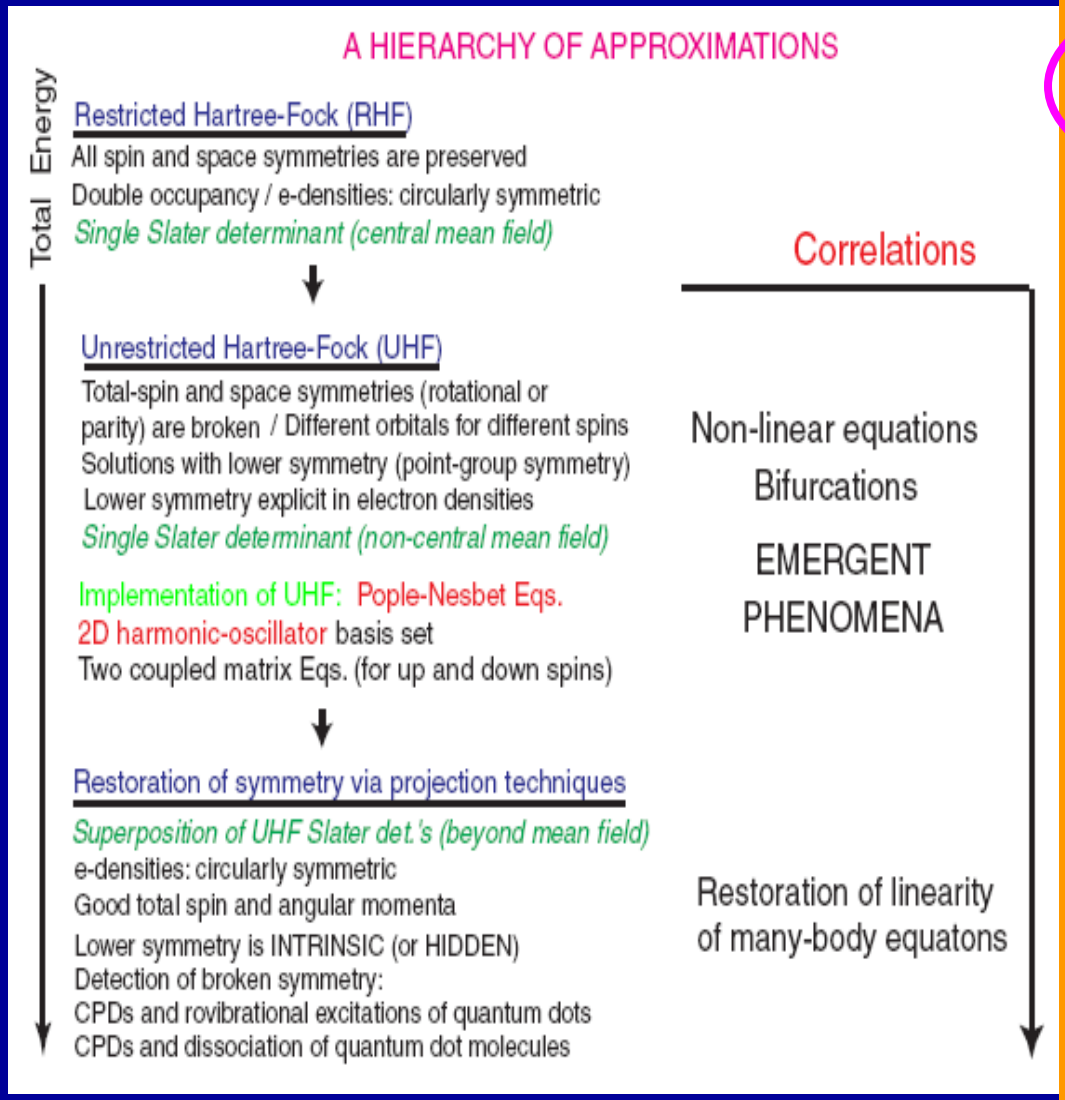
RESOLUTION OF SYMMETRY DILEMMA:

RESTORATION OF BROKEN SYMMETRY BEYOND MEAN FIELD (Projection)!

- Per-Olov Löwdin
  (Chemistry - Spin)
- R.E. Peierls and J. Yoccoz
  (Nuclear Physics – *L, rotations*)

WAVE-FUNCTION BASED APPROACHES

TWO-STEP METHOD



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)*

Mean-field broken-symmetry states

Bosons (delta): Different orbitals (Permanent)

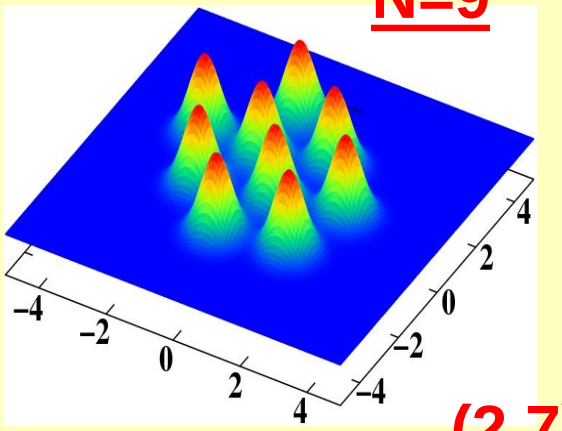
$$|\Phi_N^{\mathrm{UBHF}}\rangle \propto$$

$$\sum_{P(i_m)} \varphi_1(\mathbf{r}_{i_1})\varphi_2(\mathbf{r}_{i_2})\ldots\varphi_N(\mathbf{r}_{i_N})$$

$$\varphi_j(\mathbf{r}) \equiv \frac{1}{\sqrt{\pi}\Lambda}\exp\left[\frac{(\mathbf{r}-\mathbf{R}_j)^2}{2\Lambda^2} - i\mathbf{r}\cdot(\mathbf{Q}\times\mathbf{R}_j)\right]$$

$$\Lambda \equiv \sqrt{\hbar/(2m\Omega)} \qquad \mathbf{Q} \equiv \hat{\mathbf{z}}/(2\Lambda^2)$$

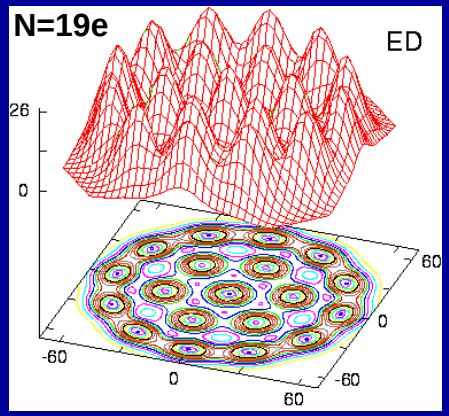
N=9



(2,7)

Electrons (Coulomb): DODS (Slater determinant)

Wigner molecule in a 2D circular QD.
Electron density (ED) from
Unrestricted Hartree-Fock.
Symmetry breaking (localized orbitals).
Concentric rings (1,6,12).



Restoration of Broken Rotational Symmetry

- To restore the good angular momentum of the wave function one can use the projection operator

$$\hat{P}_L = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{i\theta\left(L-\hat{L}\right)} = \delta(L-\hat{L})$$

- Projected wave functions can be written as a Fourier transform of unprojected wave function

$$\left|\Phi^{\mathbf{PRJ}}_{N,L}\right\rangle = \hat{P}_L\left|\Phi_N\right\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\theta \left|\Phi_N(\theta)\right\rangle e^{i\theta L}$$

Here $|\Phi_N(\theta)\rangle$ is the original UBHF permanent, rotated by an azimutal angle. The wave function $|\Phi_{PRJ}\rangle$ has not only good angular momentum, but also its energy is lower than the energy of $|\Phi_N\rangle$

Romanovsky, Yannouleas, and Landman
Phys. Rev. Lett. 93, 230405 (2004) (RBMs)

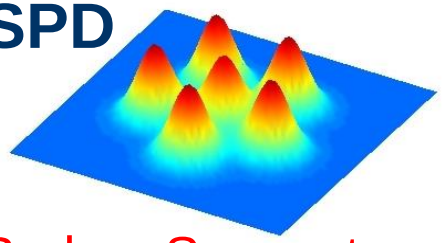
Romanovsky, Yannouleas, Baksmaty, Landman
Phys. Rev. Lett. 97, 090401 (2006) (RBMs)

Rotating Boson Molecules (Circular trap)

Ground states: Energy, angular momentum and probability densities.

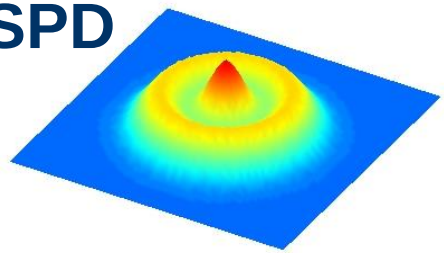
Probability densities

SPD

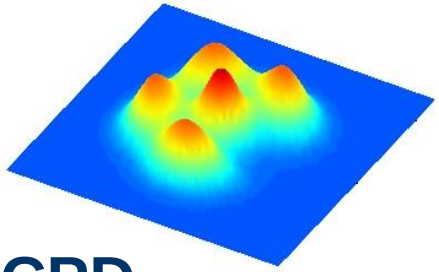


Broken Symmetry

SPD



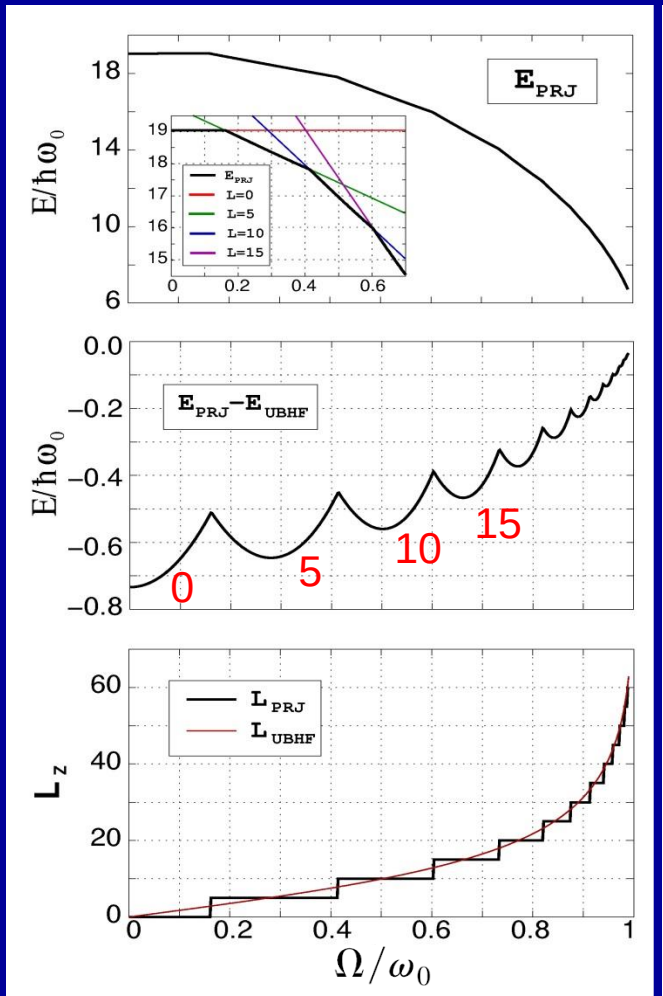
Symmetry restored



CPD

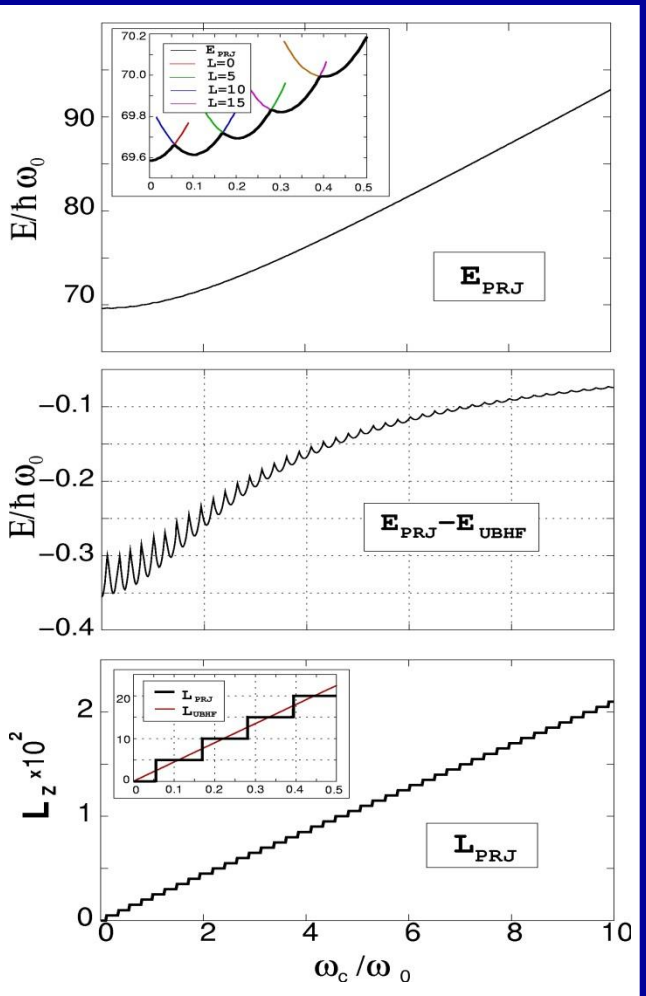
$R_\delta = 50$

Rotating Frame



R_W =10

Magnetic Field



Rotating Boson Molecules (Circular trap)

Ground states: Energy, angular momentum and probability densities.

$R_\delta = 50$

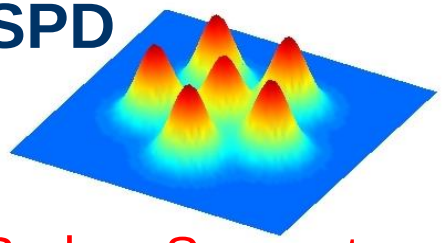
Rotating Frame

$R_W = 10$

Magnetic Field

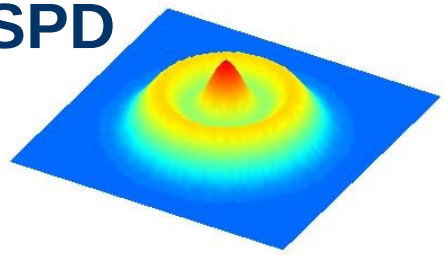
Probability densities

SPD

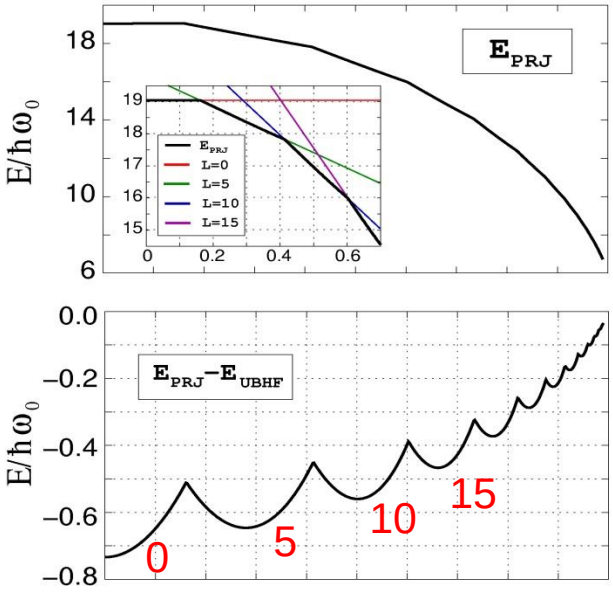


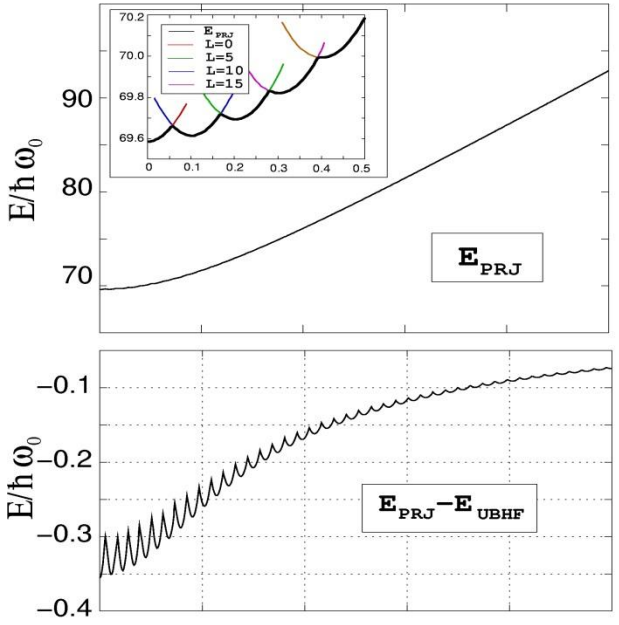
Broken Symmetry

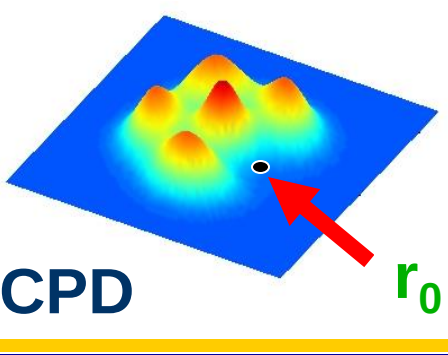
SPD



Symmetry restored







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

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

EXD/ N=12/ Lowest Landau Level/ High B/ Floppy Rotor

(3,9)

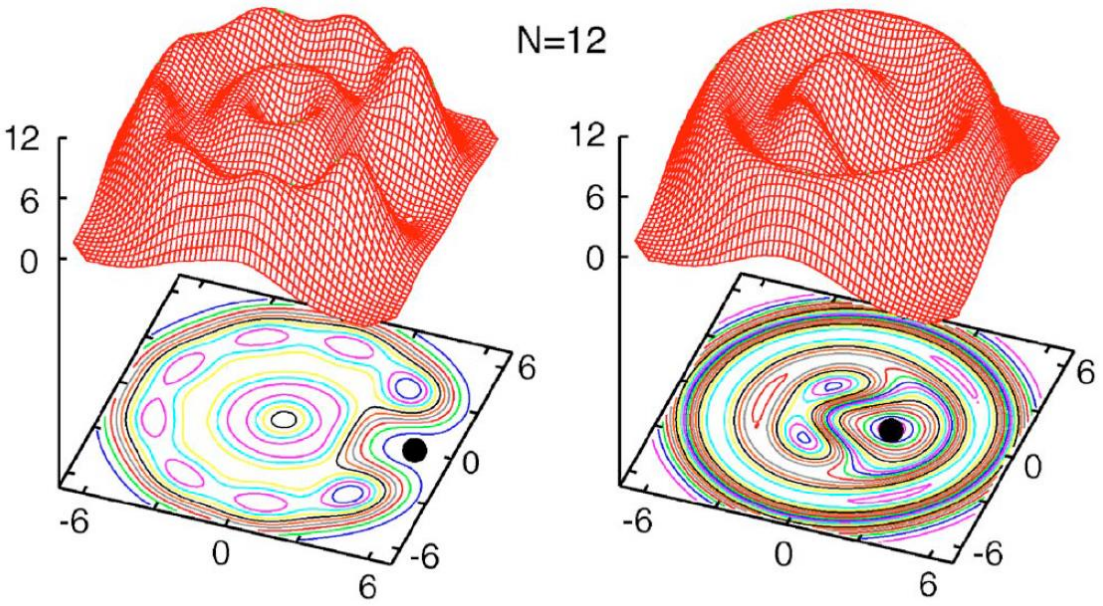


FIG. 11. (Color online) CPDs for $N=12$ electrons and with angular momentum $L=132$ ($\nu=1/2$) calculated with EXD in the lowest Landau level. The electrons are arranged in a (3,9) structure. The observation point (solid dot) is placed on the outer ring at $r_0=5.22l_B$ (left frame), and on the inner ring at $r_0=1.87l_B$ (right frame). Lengths in units of l_B. CPDs (vertical axes) in arbitrary units.

Yuesong Li, Y&L, PRB **73**, 075301 (2006)

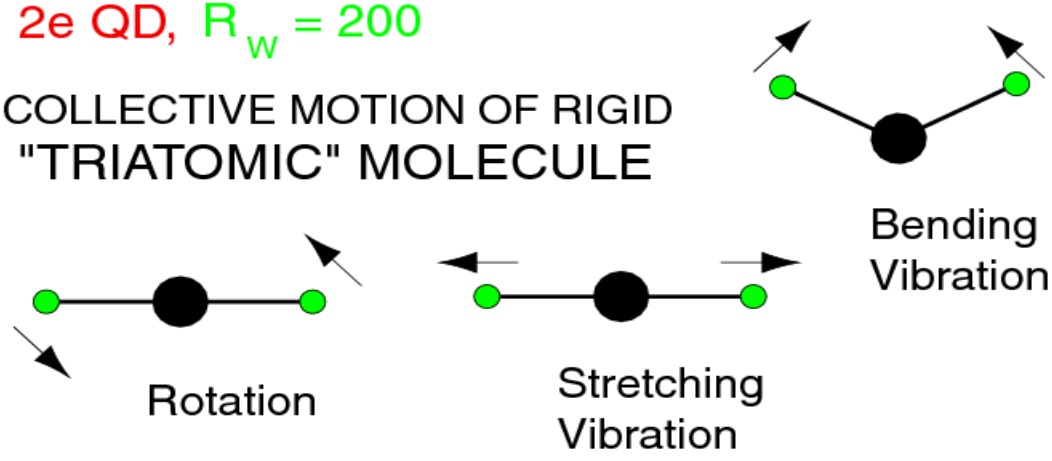
Quantum Dot Helium

Exact

Y&L, PRL 85, 1726 (2000)

2e QD, $R_W = 200$

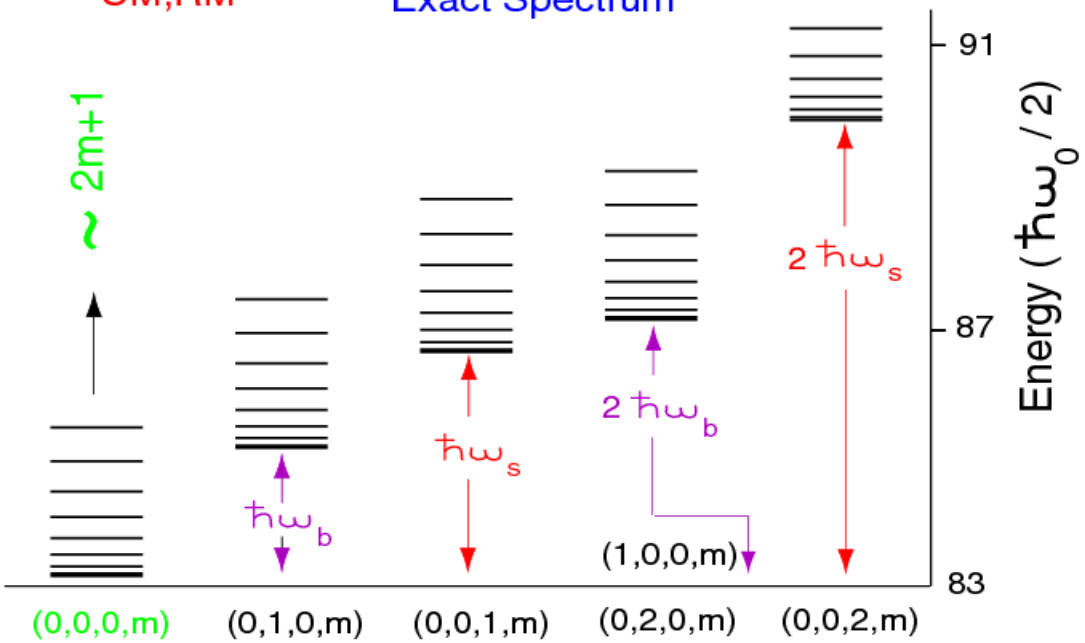
COLLECTIVE MOTION OF RIGID "TRIATOMIC" MOLECULE



$$E_{NM,nm} = Cm^2 + (n+1/2)\,\hbar\omega_s + (2N+M+1)\,\hbar\omega_b$$

CM,RM

Exact Spectrum



RIGID ROTOR

B=0

Natural Helium Doubly excited States/ Kellman/Herrick Phys. Rev. A **22**, 1536 (1980).

TWO-STEP METHOD

SECOND STEP:
RESTORATION OF SYMMETRIES VIA PROJECTION

TOTAL SPIN:

$$P_s \equiv \prod_{s' \neq s} \frac{S^2 - s'(s'+1)\hbar^2}{[s(s+1) - s'(s'+1)]\hbar^2}$$

$$S^2 \Phi_{\mathrm{UHF}} = \hbar^2 \left[(N_\alpha - N_\beta)^2/4 + N/2 + \sum_{i<j} \varpi_{ij} \right] \Phi_{\mathrm{UHF}}$$

ϖ_{ij} interchanges spins

Two electrons in a DQD:

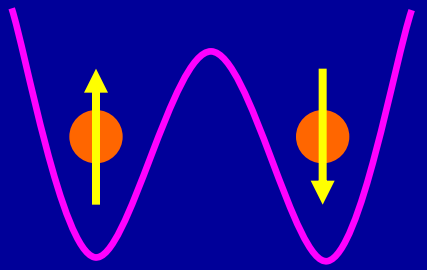
$$\Psi^s_{\mathrm{GVB}}(1,2) = n_s \sqrt{2} P_0 \Psi_{\mathrm{UHF}}(1,2)$$ ← singlet

$$2\sqrt{2} P_0 \Psi_{\mathrm{UHF}}(1,2) = (1 - \varpi_{12}) \sqrt{2} \Psi_{\mathrm{UHF}}(1,2)$$
$$= |u(1)\bar{v}(2)\rangle - |\bar{u}(1)v(2)|.$$ two det.'s

GVB, Generalized Valence Bond
GHL, Generalized Heitler London

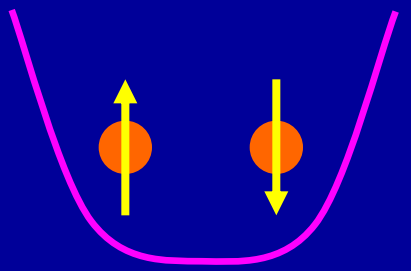
Y&L, Eur. Phys. J. D 16, 373 (2001)
Int. J. Quantum Chem. 90, 699 (2002)

DQD



localized orbitals

Elongated QD



No circular symmetry

Excitation spectrum of (elliptic) Anisotropic Quantum Dot Helium (Pinned WM)

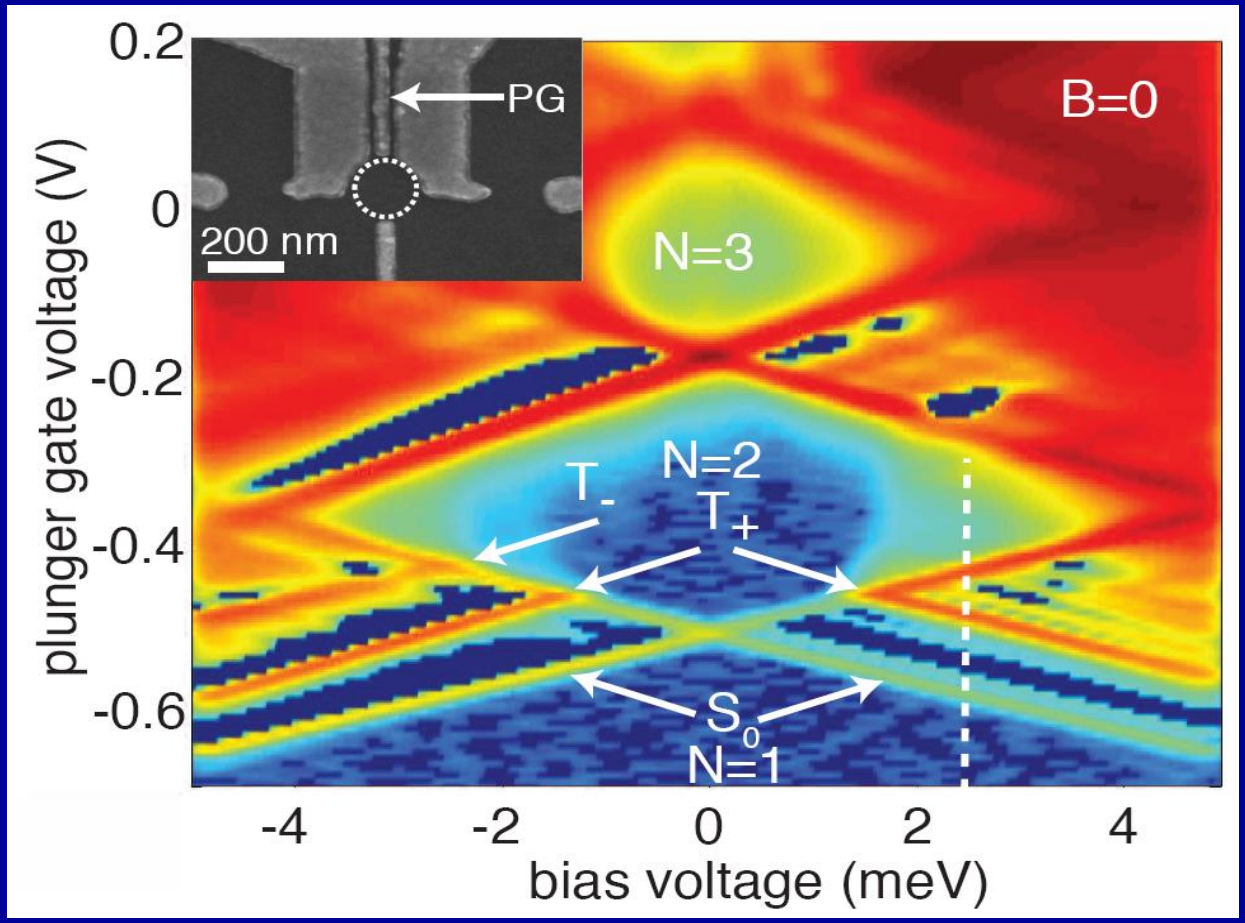
C. Ellenberger et al., Phys. Rev. Lett. **96,** 126806 (2006)

(No Zeeman splitting)

N=2e

η= 0.72

Single QD ETH Zurich (K. Ensslin, Th. Ihn…)

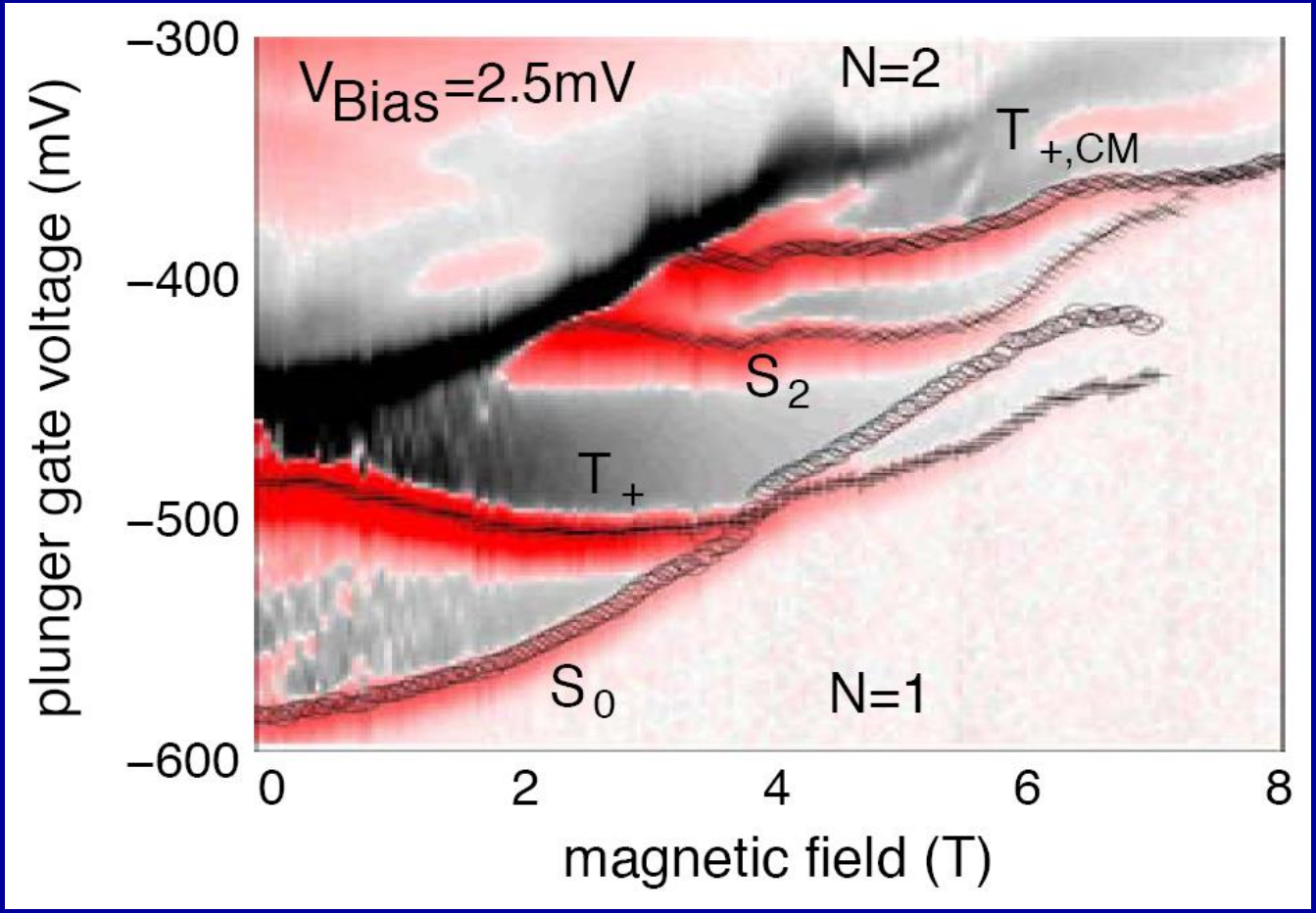


Excitation spectrum of (elliptic) Anisotropic Quantum Dot Helium (Pinned WM)

C. Ellenberger et al., Phys. Rev. Lett. **96,** 126806 (2006)

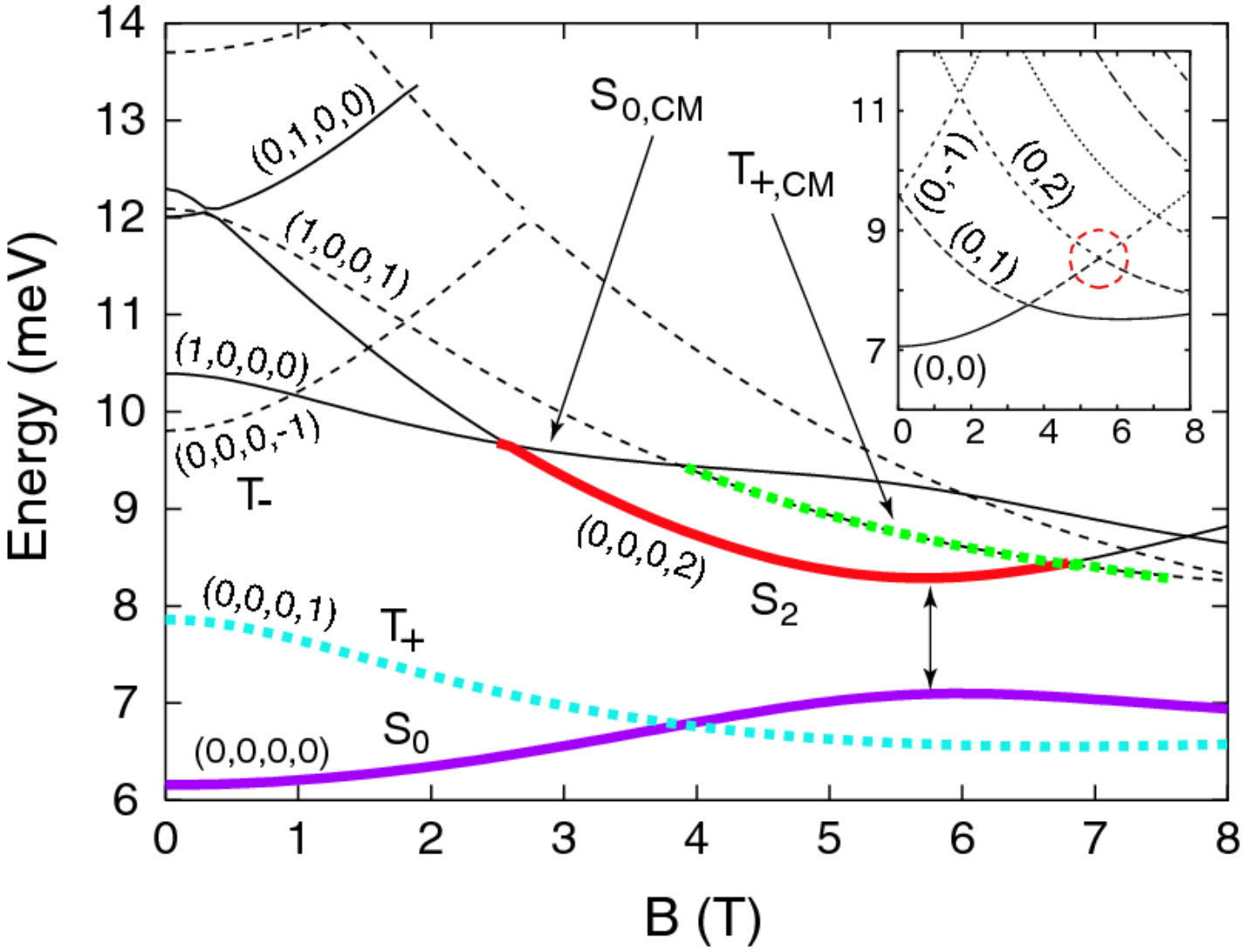
(No Zeeman splitting)

ETH Zurich single QD



ETH single QD

EXD = Exact diagonalization



$$\mathcal{H} = H(\mathbf{r}_1) + H(\mathbf{r}_2) + \gamma e^2/(\kappa r_{12})$$

4.23 meV

5.84 meV

$$H(\mathbf{r}) = T + \frac{1}{2}m^*(\omega_x^2 x^2 + \omega_y^2 y^2) + \frac{g^*\mu_B}{\hbar}\mathbf{B}\cdot\mathbf{s}$$

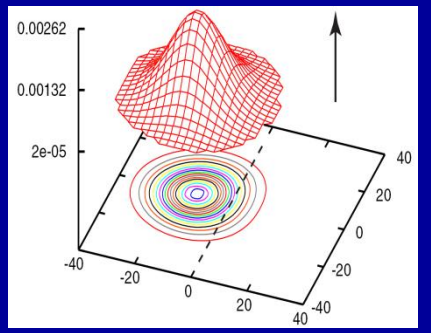
N=2e

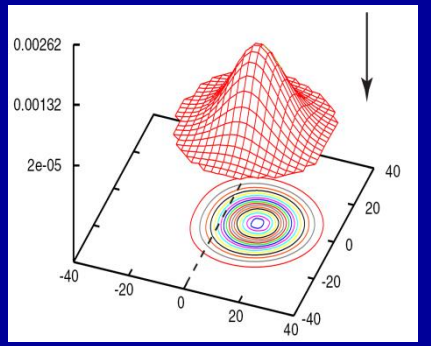
$$T = (\mathbf{p} - e\mathbf{A}/c)^2/2m^*, \text{ with } \mathbf{A} = 0.5(-By, Bx, 0)$$

B=3.8 T

UHF $\Psi_{\mathrm{UHF}}(1\uparrow, 2\downarrow) \equiv |u_L(1\uparrow)u_R(2\downarrow)\rangle$

$$u_L(1\uparrow) \equiv u_L(\mathbf{r}_1)\alpha(1) \text{ and } u_R(2\downarrow) \equiv u_R(\mathbf{r}_2)\beta(2)$$





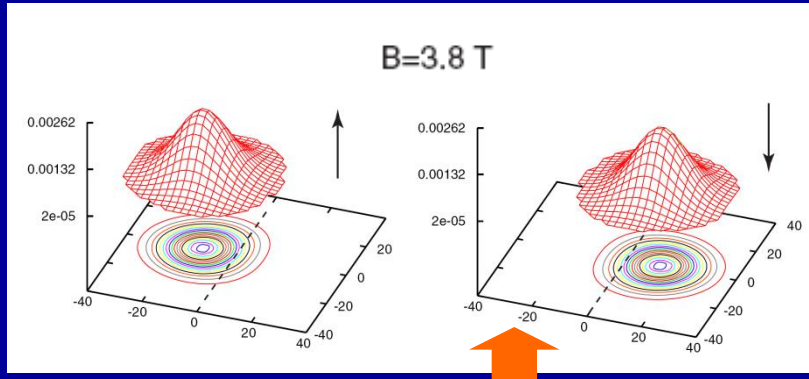
$$\Psi^{s,t}_{\mathrm{GHL}}(\mathbf{r}_1, \mathbf{r}_2) \propto \left(u_L(\mathbf{r}_1)u_R(\mathbf{r}_2) \pm u_L(\mathbf{r}_2)u_R(\mathbf{r}_1)\right)\chi^{s,t}$$

GHL $\chi^{s,t} = (\alpha(1)\beta(2) \mp \alpha(2)\beta(1))$ **Entangled**

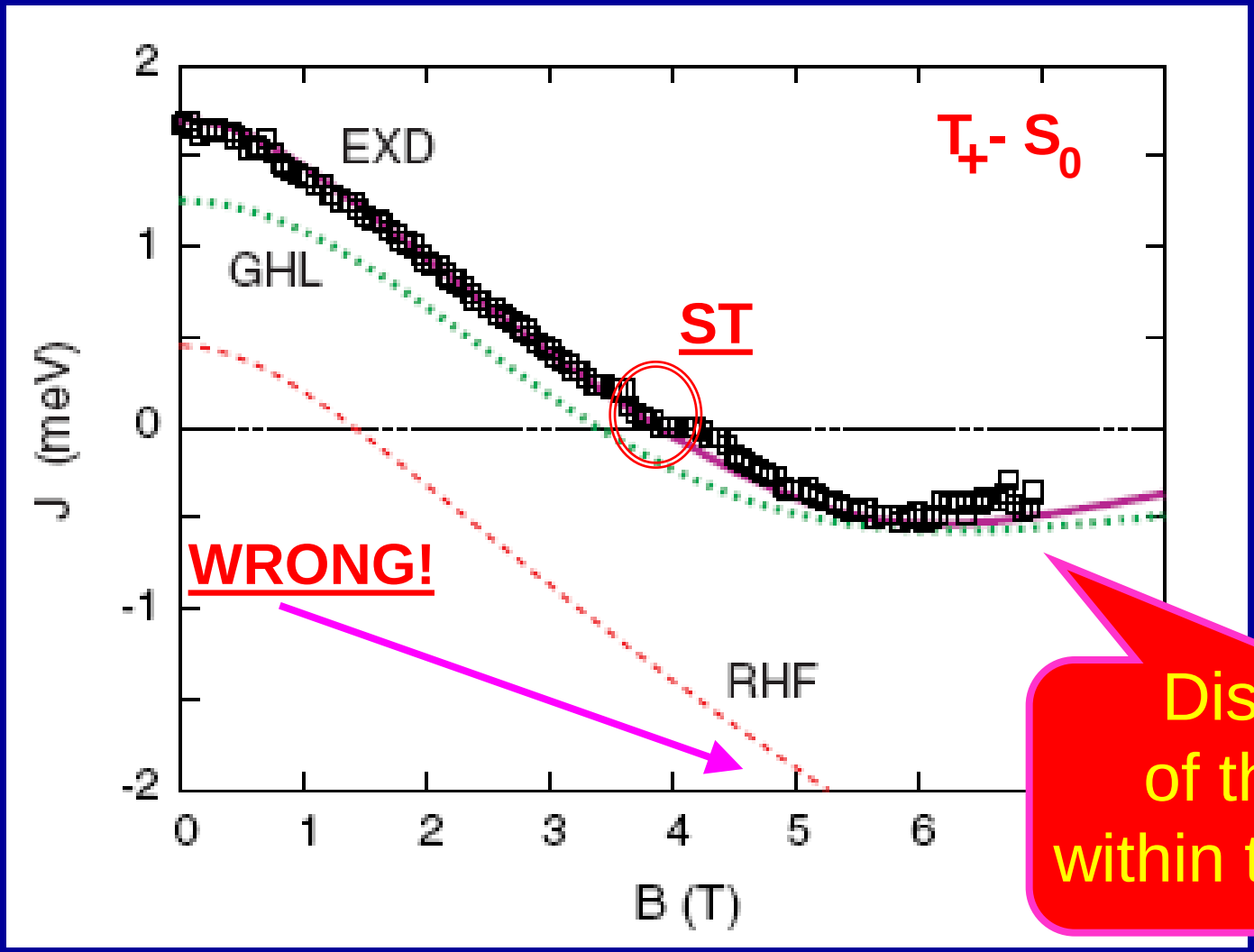
ETH single QD

hwx=4.23 meV; hwy=5.84 meV;

m*=0.070; κ=12.5; γ=0.86



UHF broken symmetry orbitals used to construct the GHL wave function



Dissociation of the 2e WM within the single QD

Three electron anisotropic QD

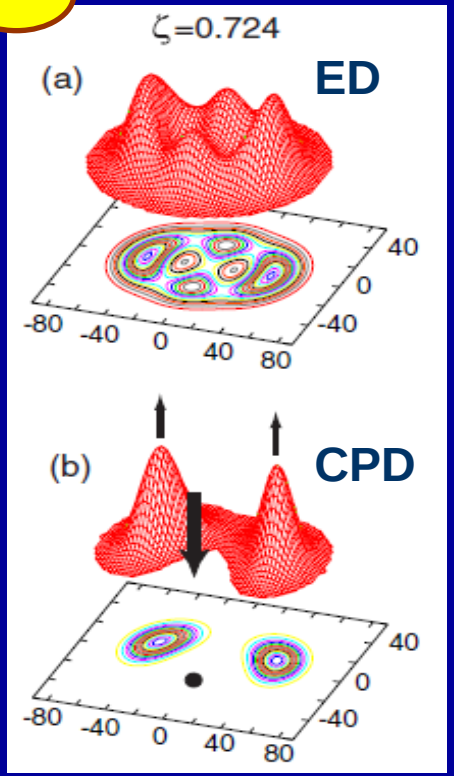
Method: ***Exact Diagonalization (EXD)***

Anisotropic confinement

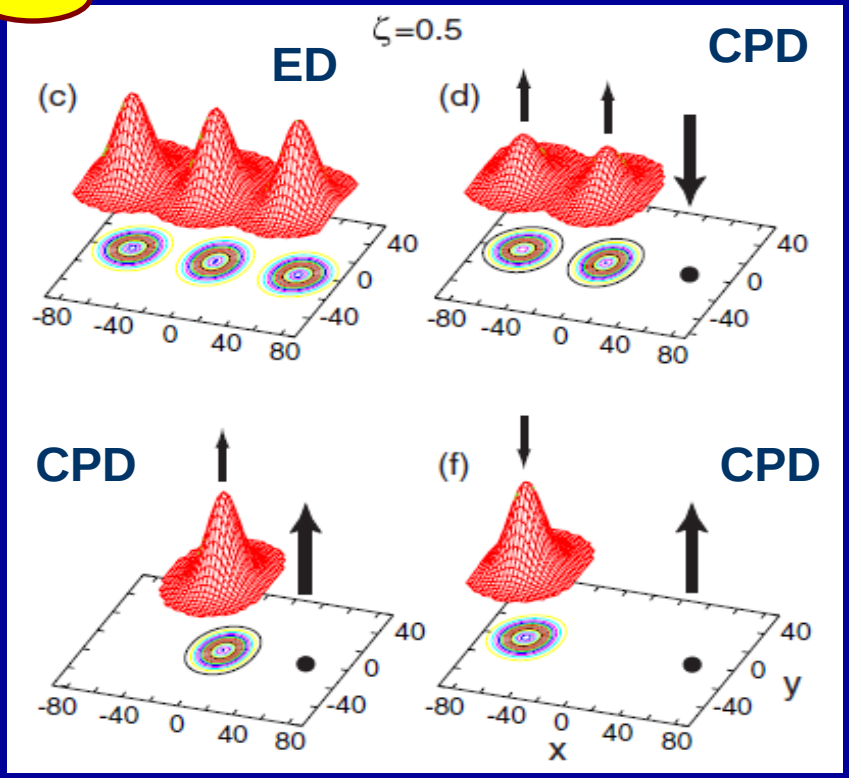
Quantum Crystallite

Electron Density (ED)

(spin resolved) Conditional Probability Distribution (CPD)



κ=1



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

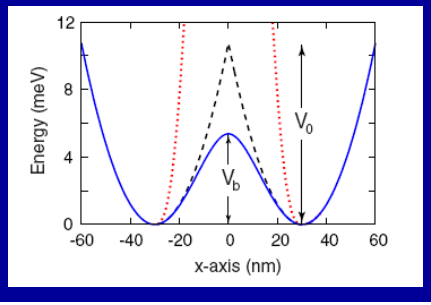
EXD wf (½, ½; 1) ~ $|\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\rangle$

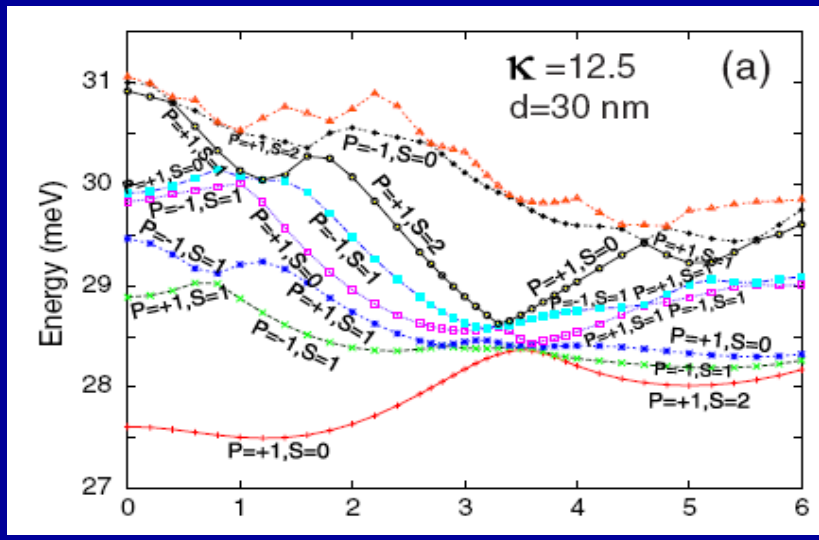
Entangled three-qubit W-states

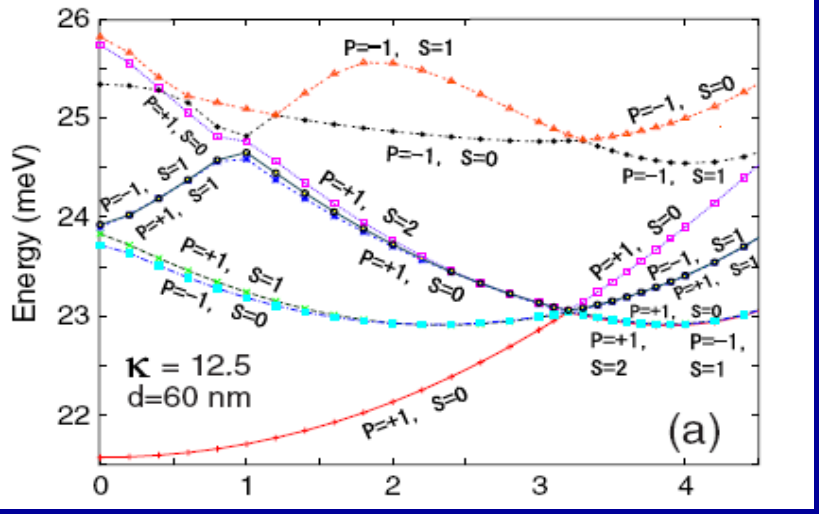
Quantum Dot Helium Molecule

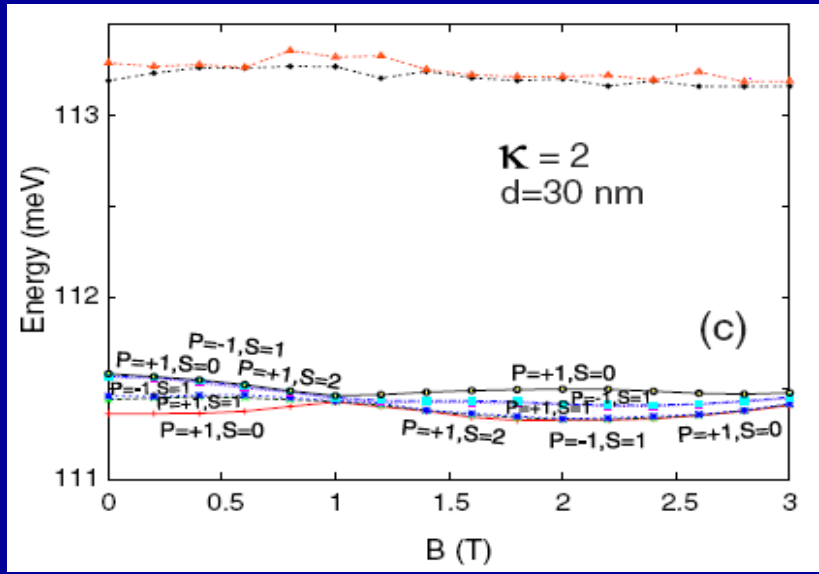
Ying Li, Y&L, Phys. Rev. B 80, 045326 (2009)

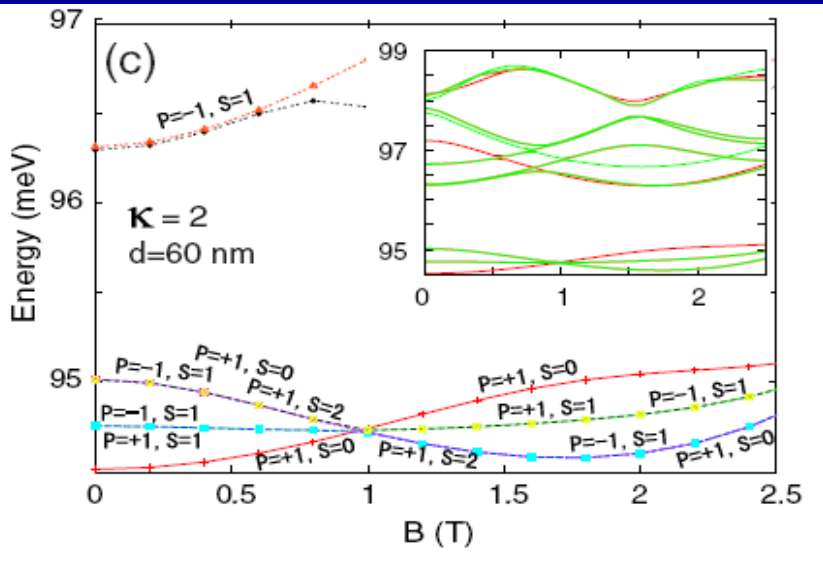
EXD calculation







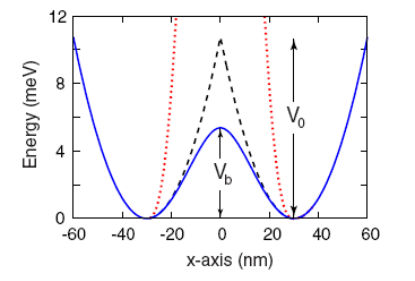


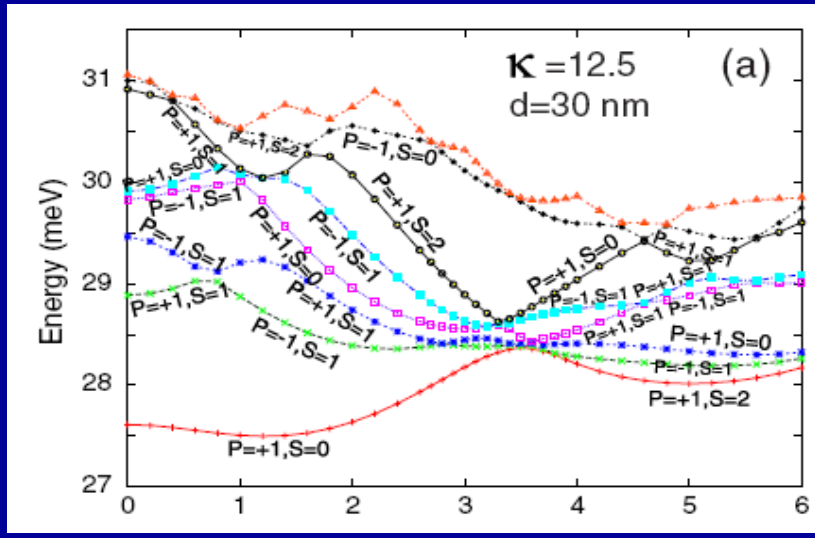


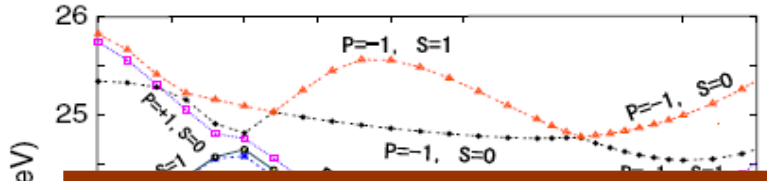
Quantum Dot Helium Molecule

Ying Li, Y&L, Phys. Rev. B 80, 045326 (2009)

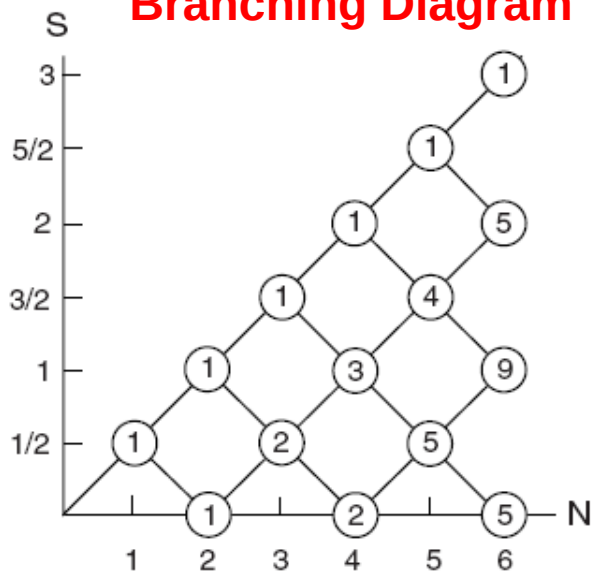
EXD calculation

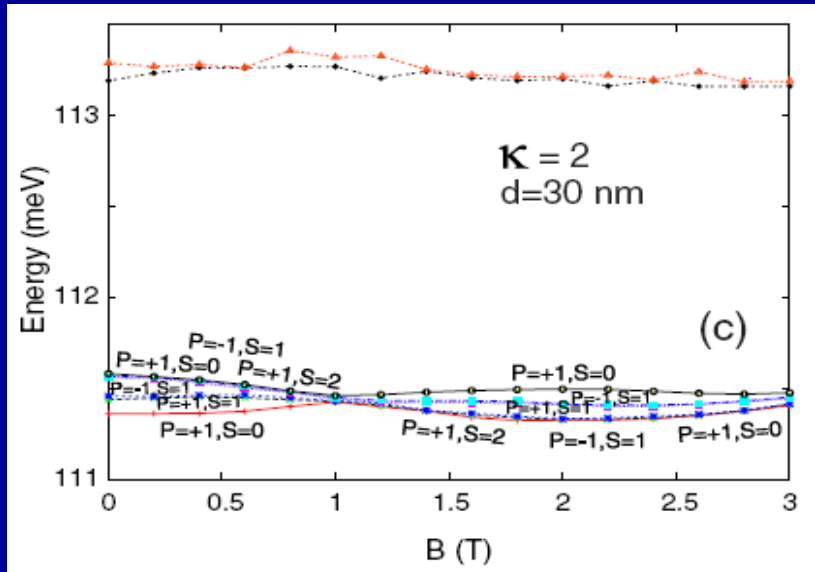


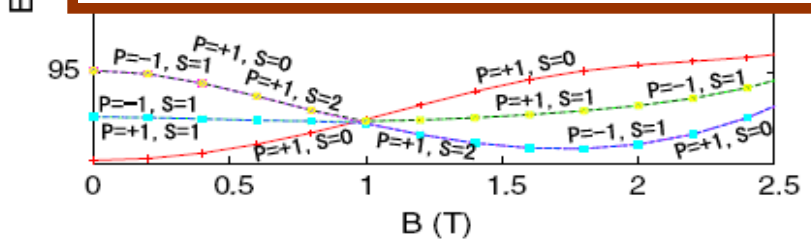




Branching Diagram







SUMMARY (Symmetry Restoration)

Under appropriate conditions, 2D electrons (and ultracold repelling bosons) exhibit localization (hidden or explicit) and organize themselves in geometric shells, forming Rotating (or pinned) Wigner Molecules (Quantum Crystallites) (semiconductor Quantum Dots, Ultracold rotating bosonic traps, Dissociation of natural molecules)

Instead of:

For electrons: organizing in electronic shells associated with a confining central potential (Cluster physics/ jellium model)

For bosons: forming a Bose-Einstein condensate

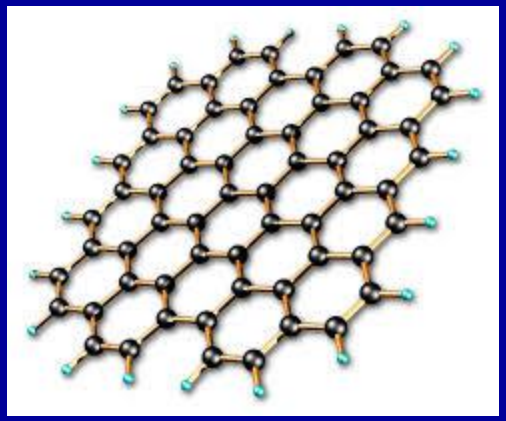
In the LLL: Rovibrational molecular theory offers alternative description to Laughlin and composite-fermion approaches for the fractional quantum Hall effect

THIRD PART

Topological states in graphene *nanorings*: Particle-physics analogies beyond the (massless and constant mass) Dirac fermion

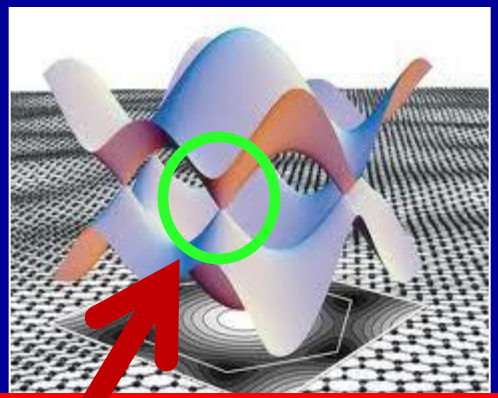
A different physical process for electron localization
Topology (geometry) of system
One-body / no e-e interaction/ fraction of e localized

Romanovsky, Yannouleas, Landman,
PRB **87**, 165431 (2013)



2D Graphene:
honeycomb lattice
Geim and Novoselov,
Nobel Prize, 2010

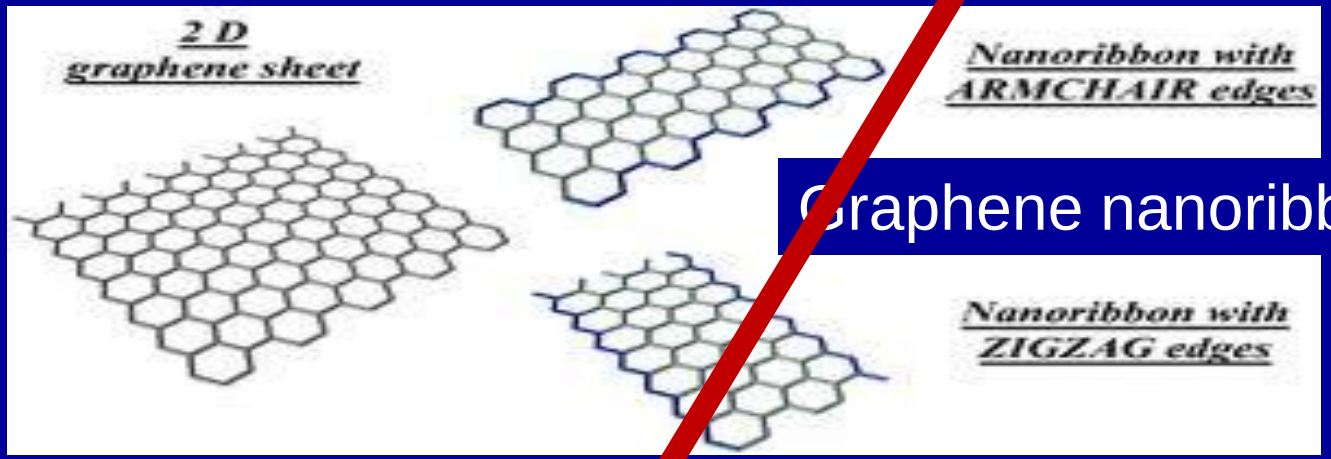
c → v_F



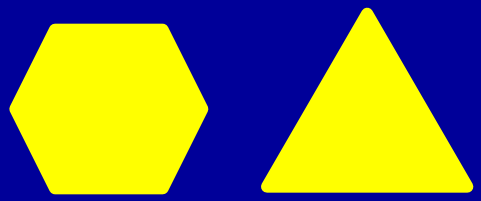
Massless Dirac-Weyl fermion

Graphene Nanosystems

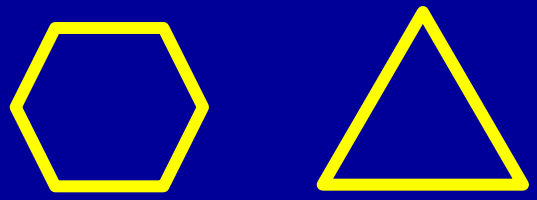
Armchair or Zigzag edge terminations



Graphene nanoribbons



Open a gap?

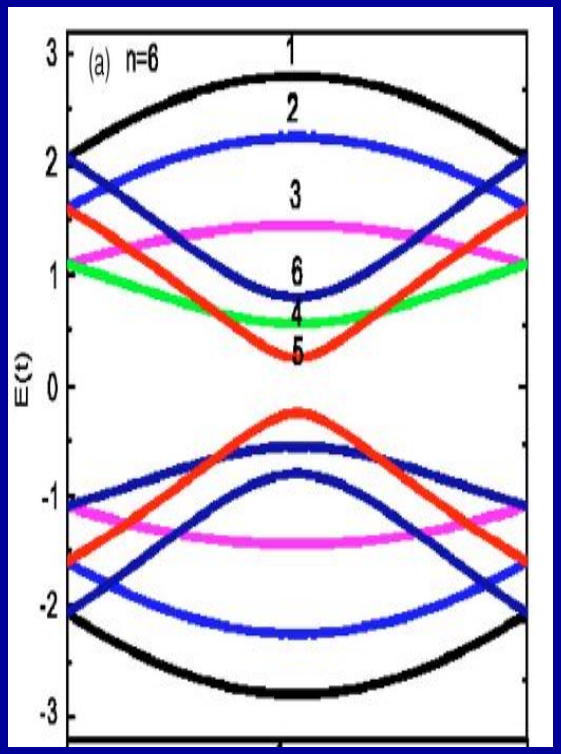


Graphene quantum dots

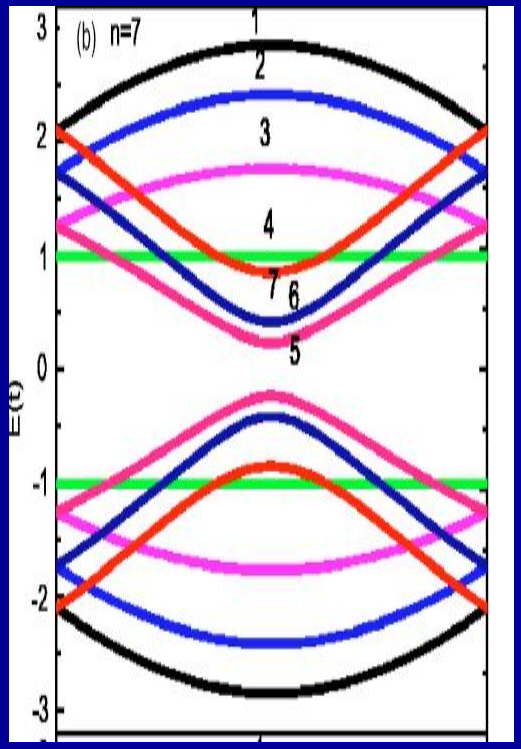
Graphene nanorings

Armchair Nanoribbons

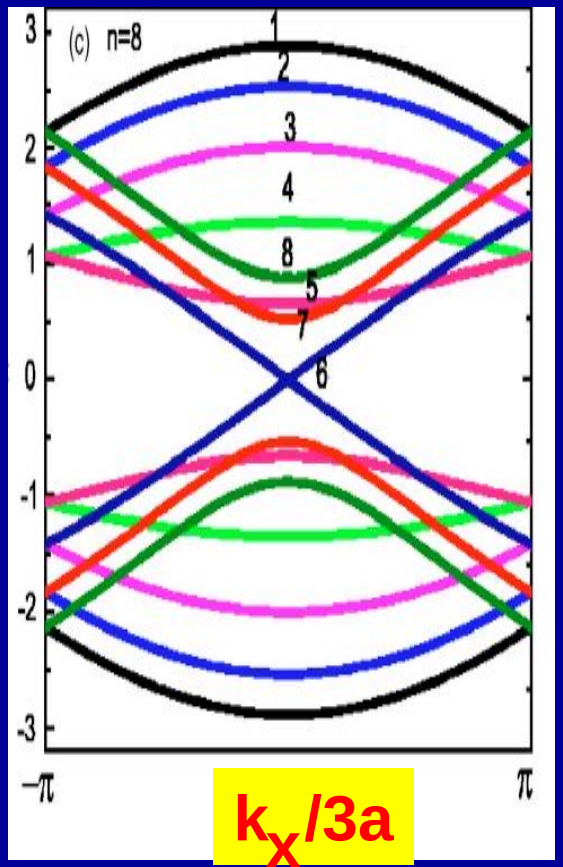
Energy (t = 2.7 eV)



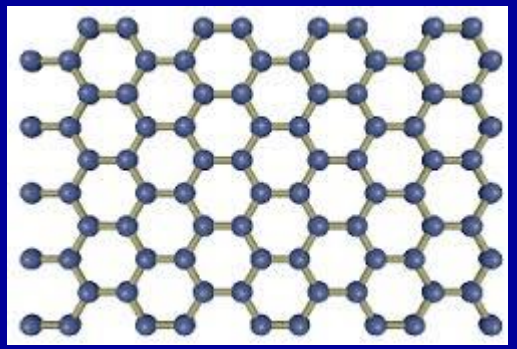
N=3m (Class I)
Semiconductor



N=3m+1 (Class II)
Semiconductor



N=3m+2 (Class III)
Metallic



N

X

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

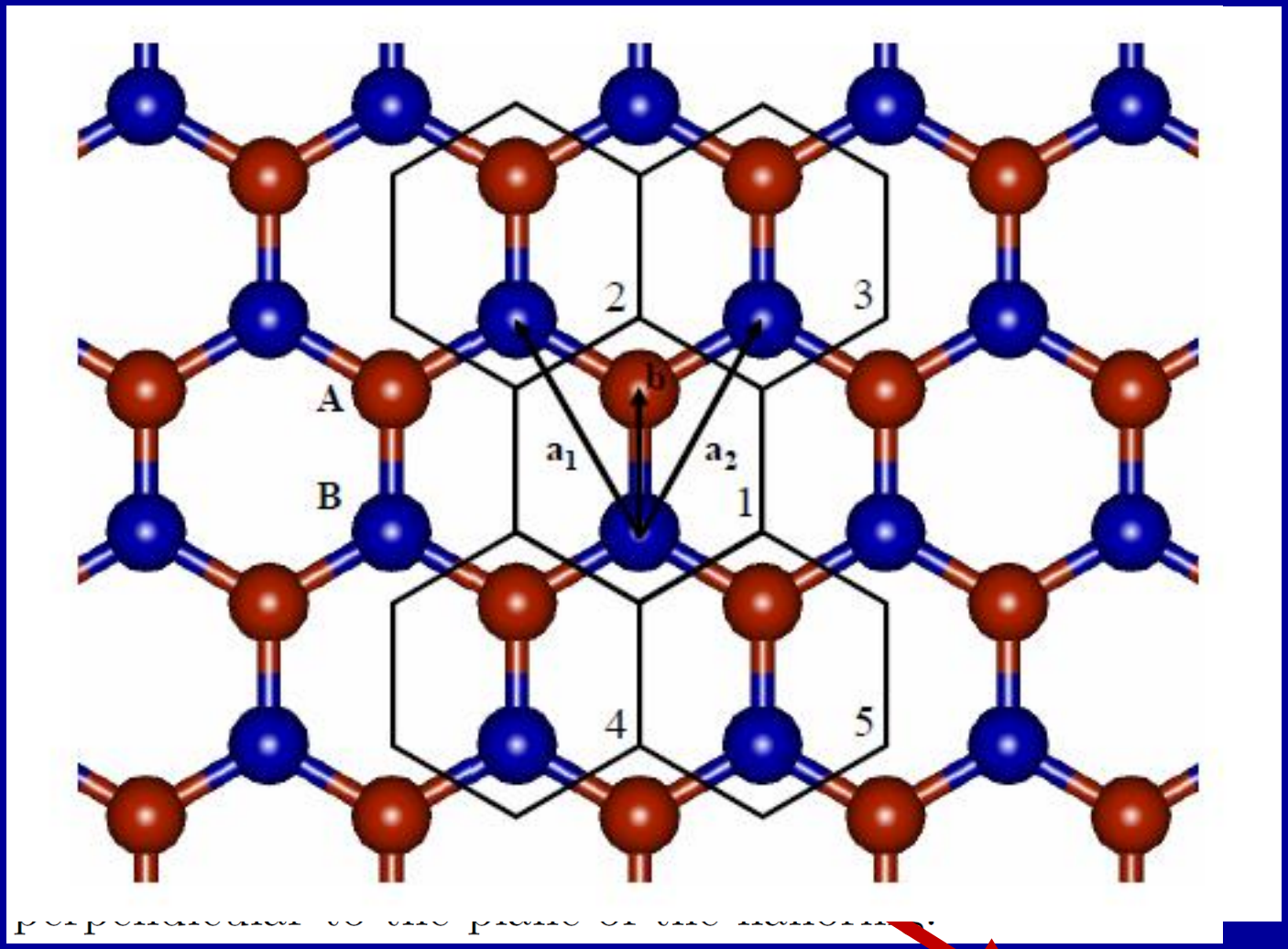
$$\tilde{t}_{ij} = t_{ij} \exp\left(\frac{ie}{\hbar c}\int_{\mathbf{r}_i}^{\mathbf{r}_j} d\mathbf{s}\cdot\mathbf{A}(\mathbf{r})\right), \qquad (2)$$

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

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

Tight-Binding (TB)



2.7 eV

1D Generalized Dirac equation

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

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

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

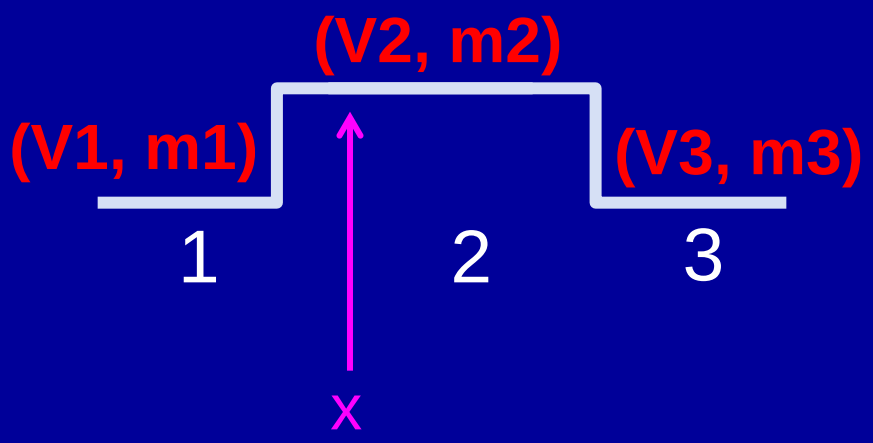
electrostatic potential

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

Dirac-Kronig-Penney Superlattice

Transfer matrix method

a single side/ 3 regions



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

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

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

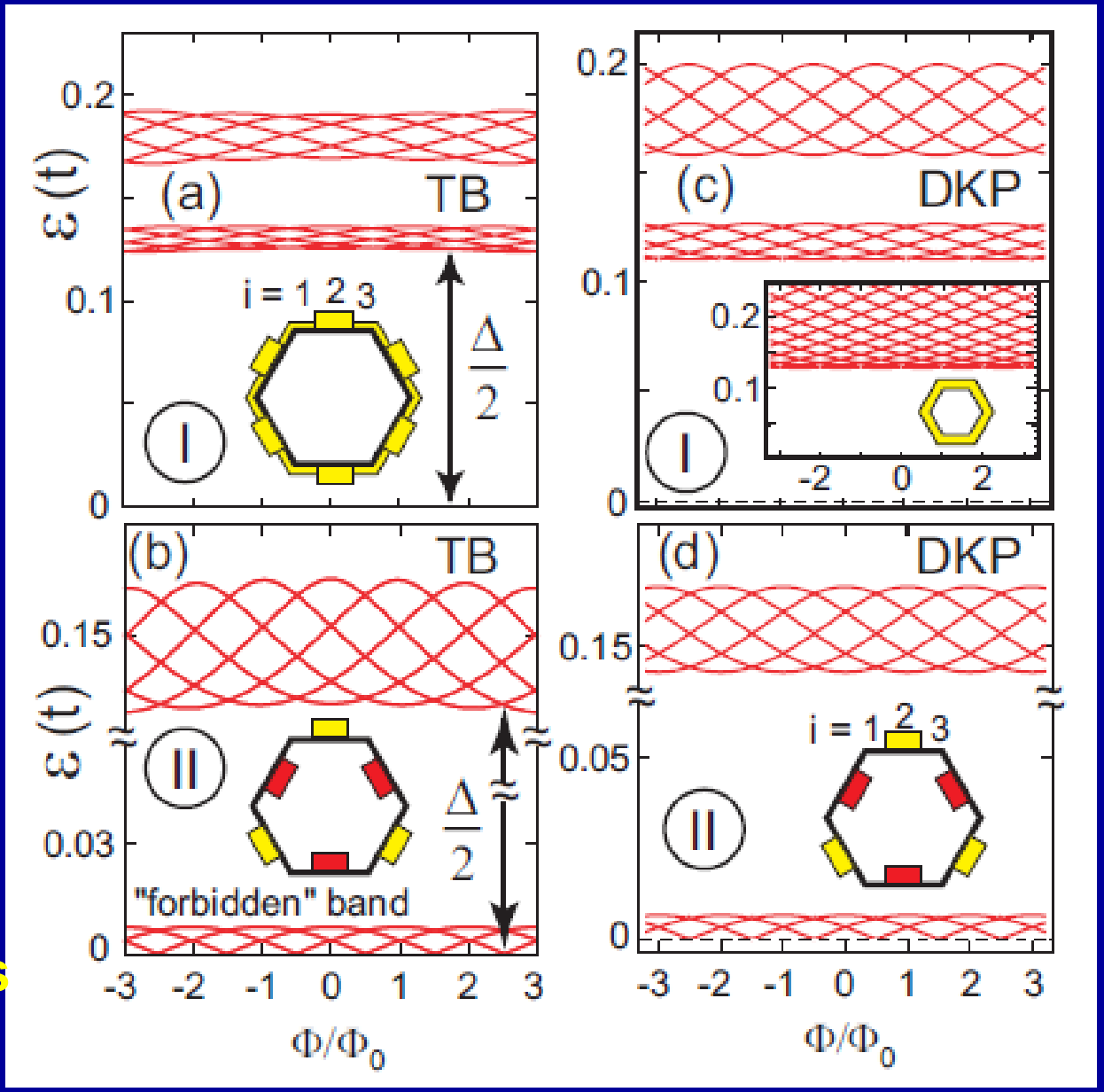
Spectra/
Rings with
semiconducting
arms

N=15 (Class I)

N=16 (Class II)

Yellow: positive mass

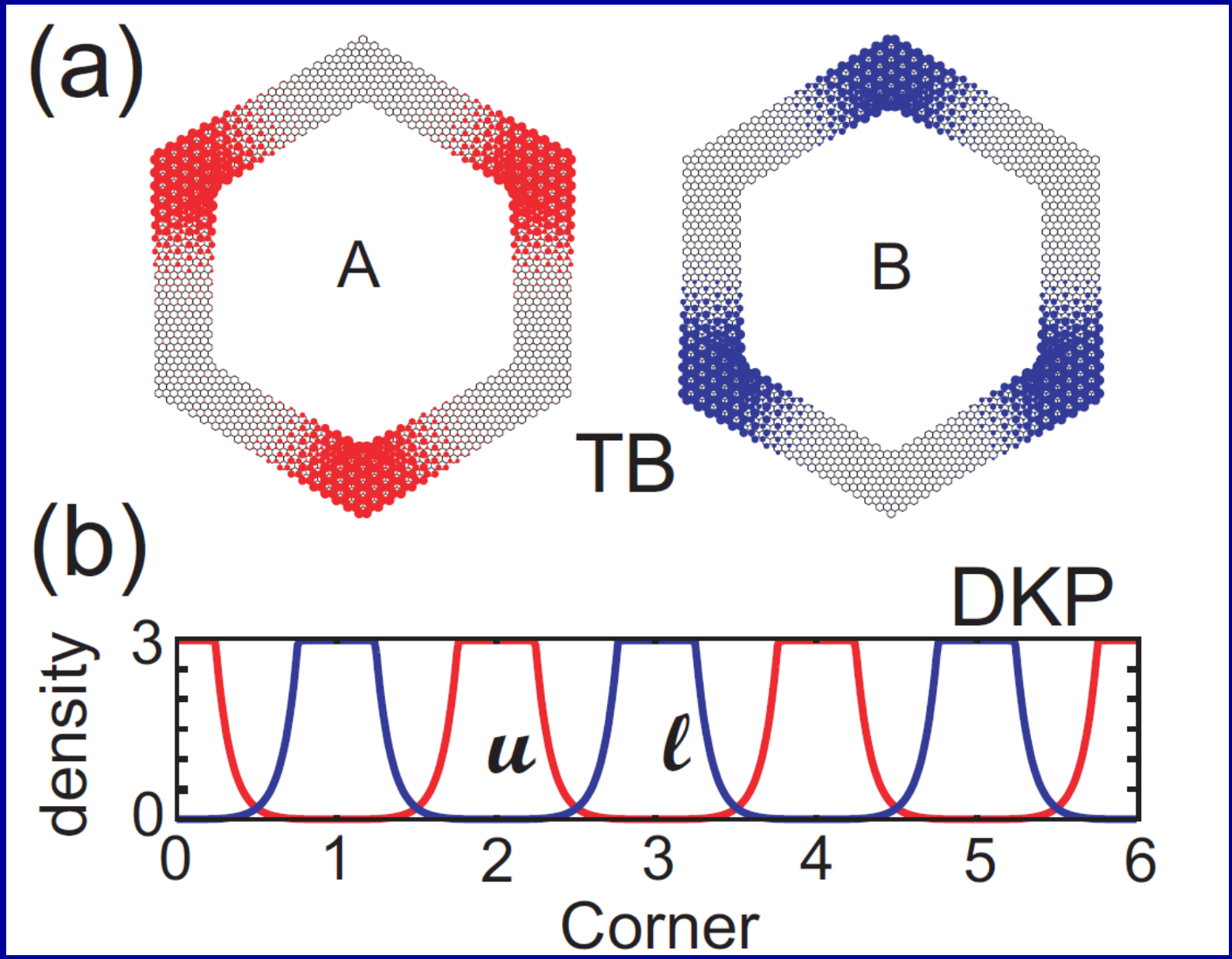
Red: negative mass



Magnetic flux (magnetic field B)

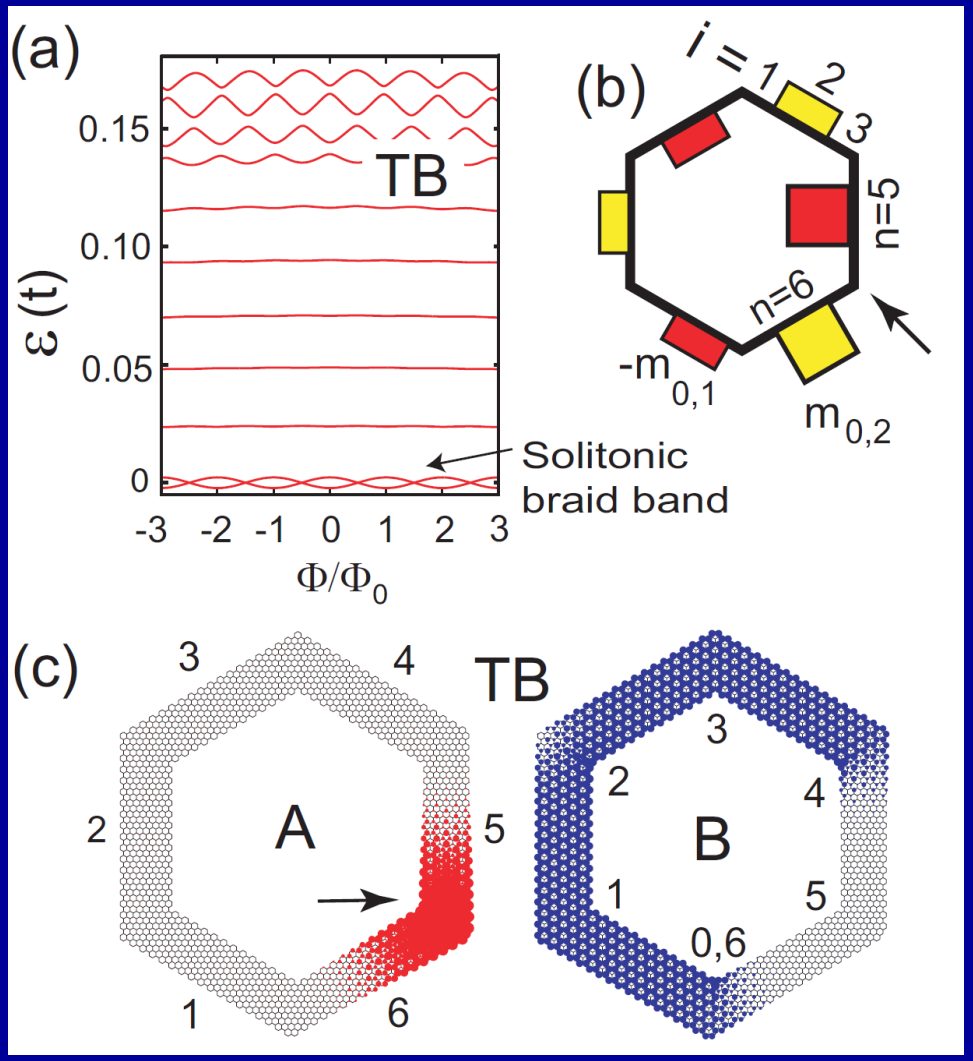
Densities for a state in the forbidden band

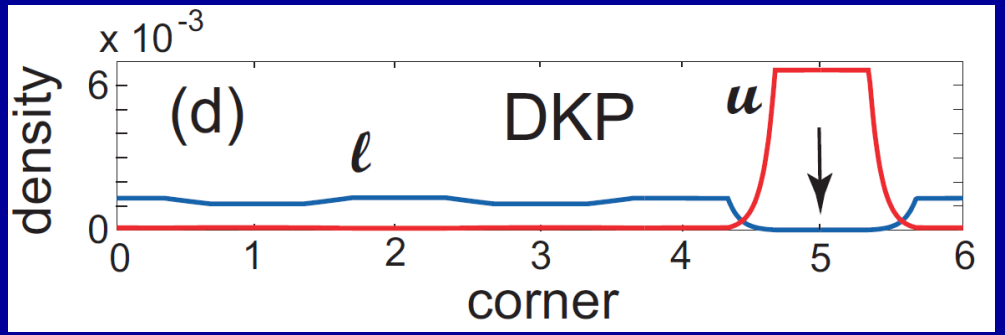
e/6 fractional charge



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

e/2
fractional charge





1D Generalized Dirac equation

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

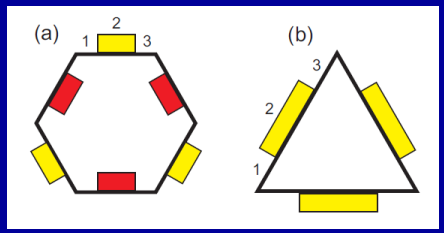
fermion

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

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

electrostatic potential

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



Relativistic quantum-field-theory Lagrangian

$$\mathcal{L} = \mathcal{L}_f + \mathcal{L}_\phi$$

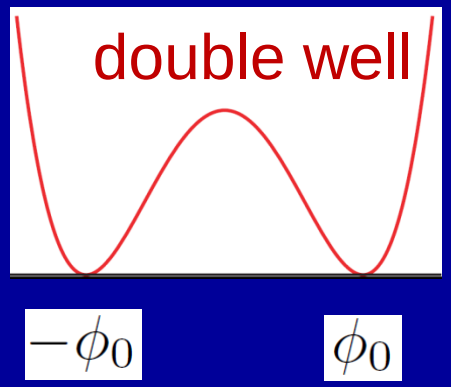
Yukawa coupling

$$\mathcal{L}_f = -i\hbar\Psi^\dagger \frac{\partial}{\partial t}\Psi - i\hbar v_F \Psi^\dagger \alpha \frac{\partial}{\partial x}\Psi - \phi\Psi^\dagger\beta\Psi$$

fermionic

scalar field

$$\mathcal{L}_\phi = -\frac{1}{2}(\frac{\partial\phi}{\partial x})^2 - V(\phi) \quad + \quad V(\phi) = \frac{\xi}{4}(\phi^2 - \zeta^2)^2$$

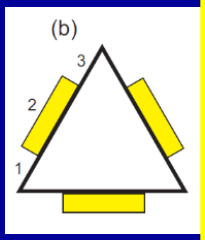


Euler-Lagrange equation

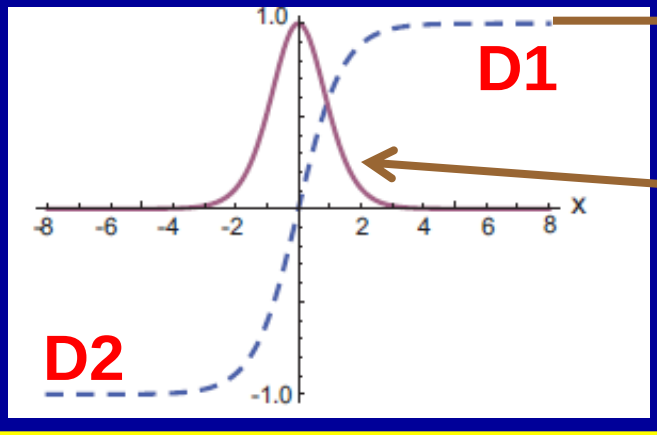
$$-\frac{\partial^2\phi}{\partial x^2} + \xi(\phi^2 - \zeta^2)\phi = 0$$

solutions

1 ϕ_0 (Symmetry breaking)/ constant mass Dirac fermion

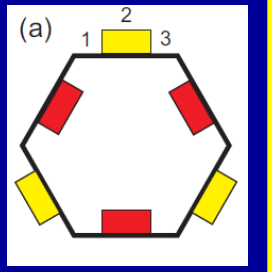


2 kink soliton/ zero-energy fermionic soliton



kink soliton

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

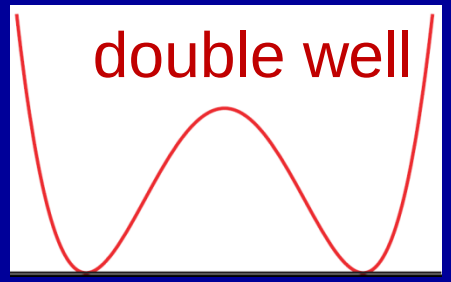


zero-energy fermionic soliton (Dirac eq.)

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

scalar field

$$\mathcal{L}_\phi = -\frac{1}{2}(\frac{\partial\phi}{\partial x})^2 - V(\phi) \quad + \quad V(\phi) = \frac{\xi}{4}(\phi^2 - \zeta^2)^2$$



Euler-Lagrange equation

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solutions

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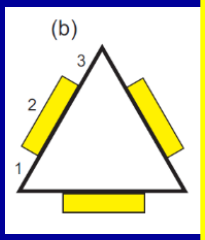
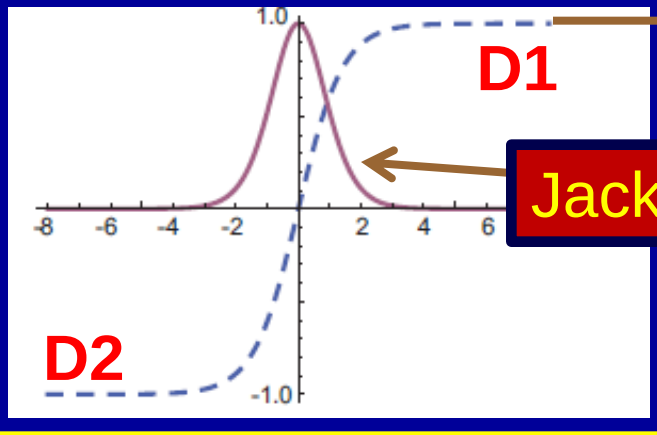
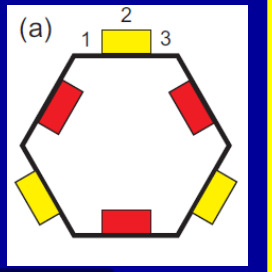


2 kink soliton/ zero-energy fermionic soliton



kink soliton

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



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

...c eq.)

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

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).