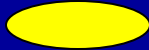


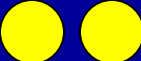
ARTIFICIAL FEW-ELECTRON SINGLE AND MOLECULAR
QUANTUM DOTS IN LOW MAGNETIC FIELDS:
ELECTRONIC SPECTRA, SPIN CONFIGURATIONS,
AND HEISENBERG CLUSTERS

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



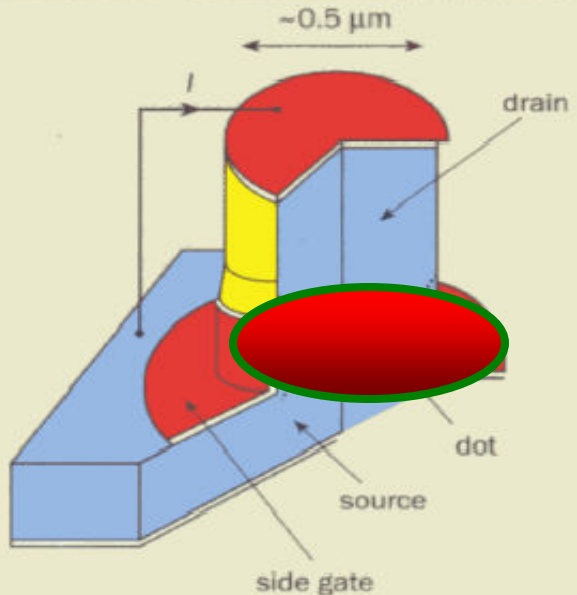
N=2e: C. Ellenberger et al, Phys. Rev. Lett. 96, 126806 (2006), 
T. Ihn et al., Int. J. Mod. Phys. B 21, 1316 (2007) (*single anisotropic dots*)

N=3e: Yuesong Li et al.: PRB 76, 245310 (2007) (*single anisotropic dots*) 

N=4e: Ying Li et al.: PRB 80, 045326 (2009) (*double quantum dots*) 

Method: Exact Diagonalization (EXD)

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

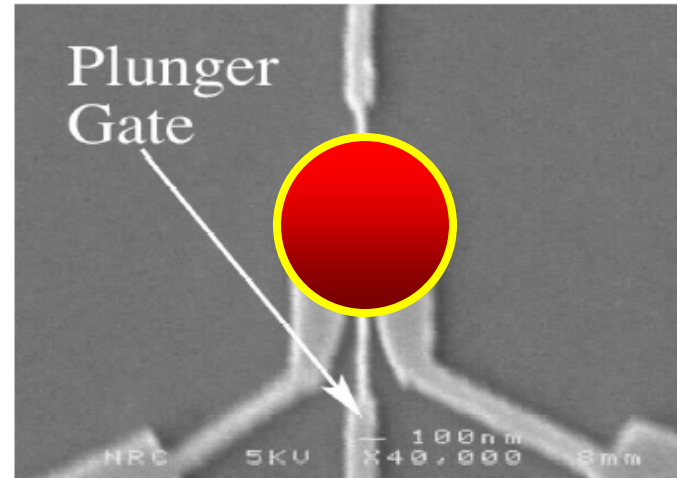
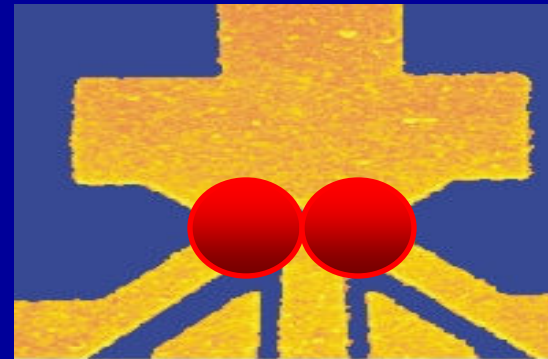


FIG. 1. SEM image of the gate geometry forming the quantum dot. This geometry enables a precisely known number of electrons ($N=0,1,2, \dots, 50$) to be trapped (Ref. 13) and produces a quasiparabolic confinement potential. Sweeping the plunger-gate voltage tunes both the shape and the chemical potential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

Lateral QD (Ottawa)



Lateral QD Molecule (Delft)

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

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

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

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

External confinement

Parabolic, single QD

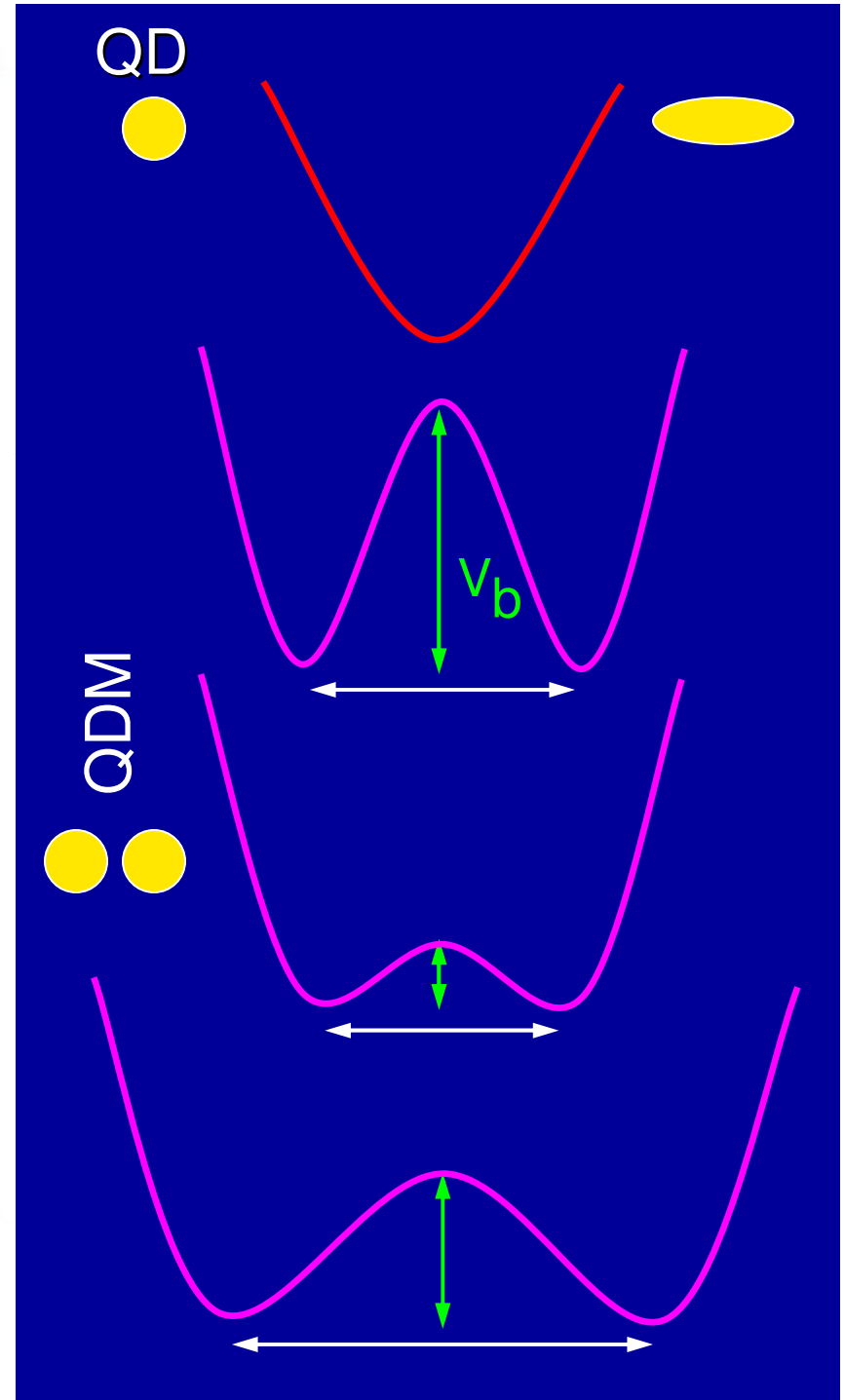
Two-center oscillator } QDM
with V_b control

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

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

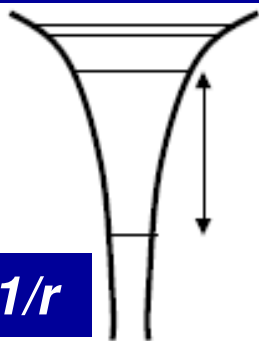
↑
Zeeman

H can be generalized to:
Multi-component systems



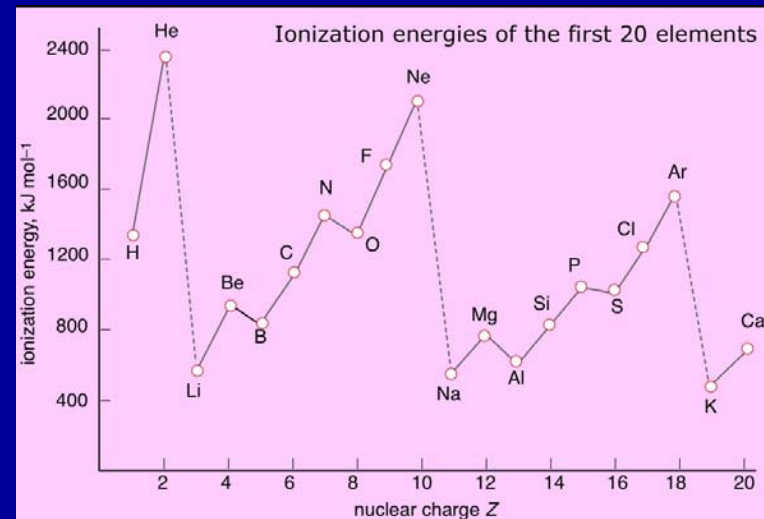
Central potential: Electronic shell effects

Natural atoms



$$V(r) \sim 1/r$$

PERIODIC TABLE OF THE ELEMENTS
CENTRAL WASHINGTON UNIVERSITY

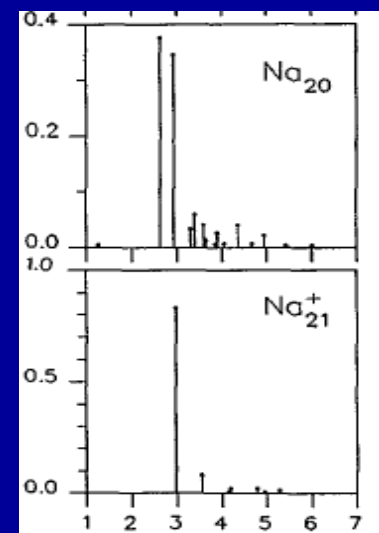
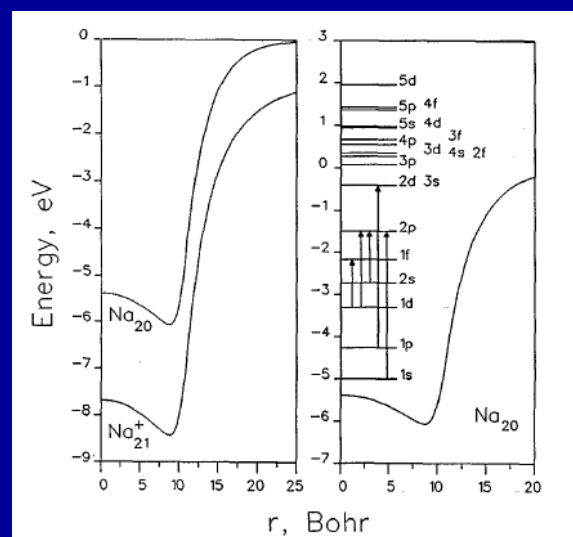


3D Clusters/Superatom: Density functional theory

Magic numbers: 2, 8, 18, 20, ...

Giant resonances/
optical response/ RPA

Yannouleas et al., PRL **63**, 255 (1989)



Wigner Crystals

DECEMBER 1, 1934

PHYSICAL REVIEW

VOLUME 46

On the Interaction of Electrons in Metals

E. WIGNER, *Princeton University*

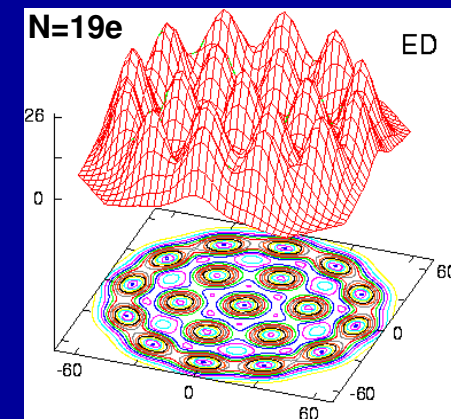
(Received October 15, 1934)

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

fact that the electrons repel 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

... electrons repel 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" ...

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



CONTROLLING PARAMETERS

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

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

κ : dielectric const. (12.9)

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

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

- **In a magnetic field, essential parameter is B itself**

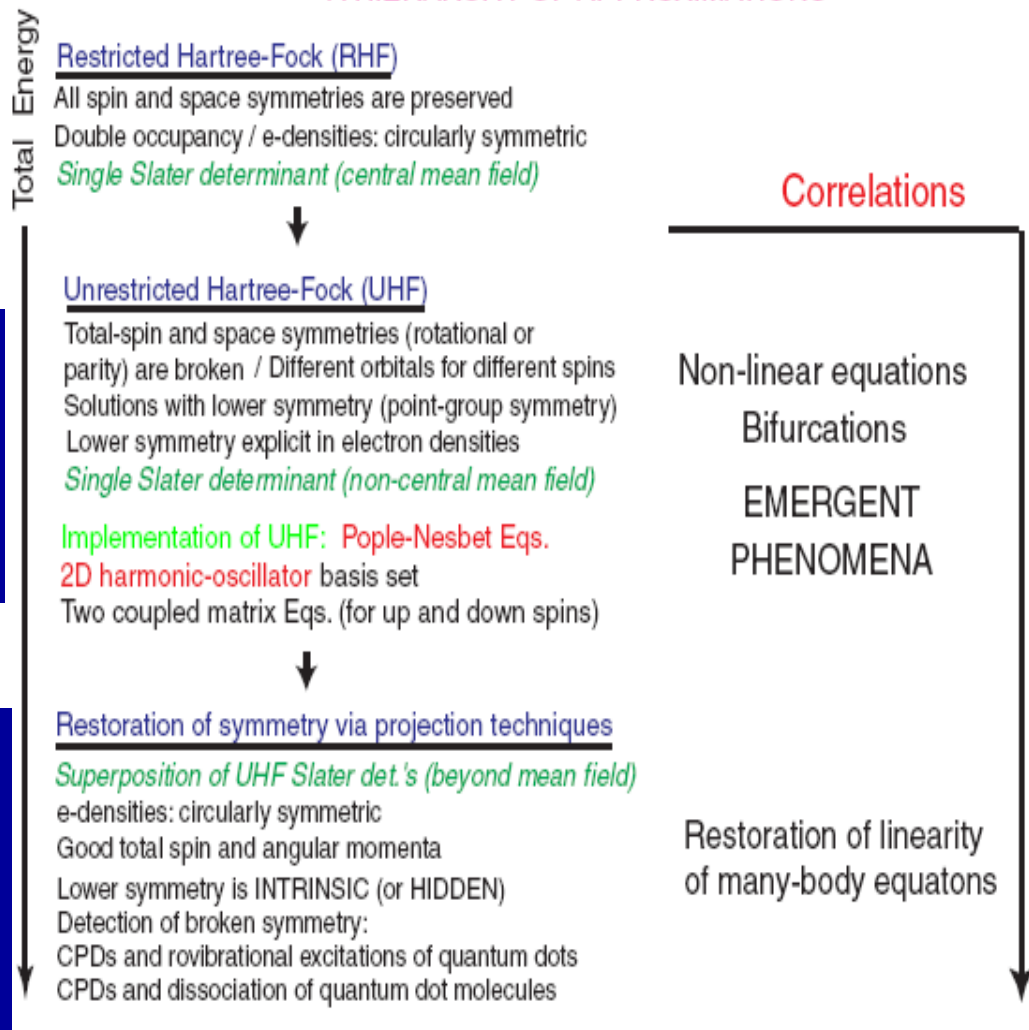
IN QDM'S: DISSOCIATION (Electron puddles, Mott transition)

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

WAVE-FUNCTION BASED APPROACHES

TWO-STEP METHOD

A HIERARCHY OF APPROXIMATIONS



Static corr.

Dynamical corr.

**EXACT
DIAGONALIZATION**

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

**Physics less
transparent
compared to
"THE TWO-STEP"**

**Pair correlation functions,
CPDs**

Applications of EXD approach **(to strongly-correlated 2D electrostatic QDs)**

- 1) Detailed description of excitation spectra
(advantage over DFT, etc...)
- 2) Description of many-body entanglement
(advantage over DFT, etc...)
- 3) Transport properties in QDs (current intensity,
phase lapses in Aharonov-Bohm interferometry)

EXD many-body wave function:

$$|\Psi_N^{\text{EXD}}(S, S_z; k)\rangle = \sum_I C_I^N(S, S_z; k) |SD(I; N, S_z)\rangle$$

$I \sim 500,000$

Slater determinant

All symmetries conserved: total L, total S, S_z

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

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

(No Zeeman splitting)

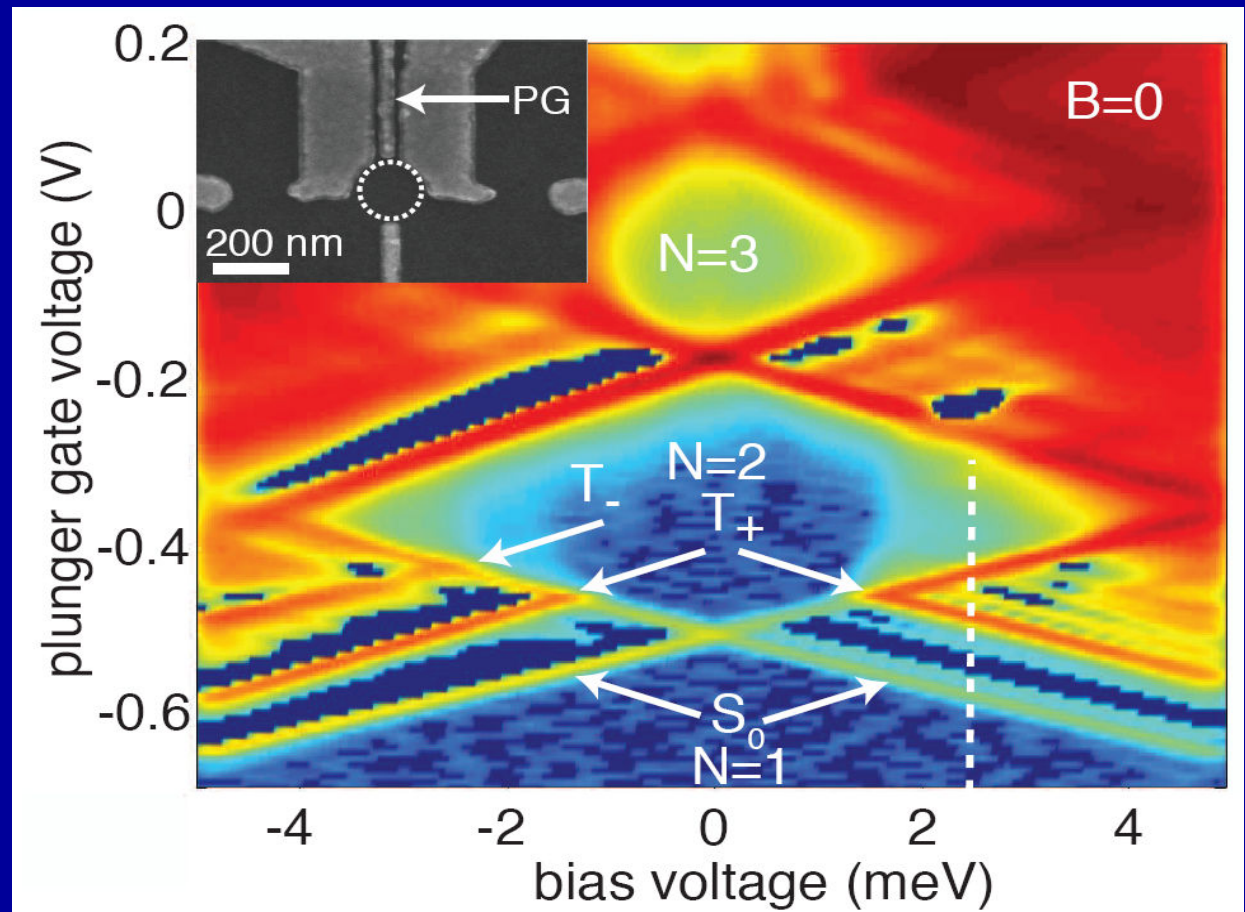
$N=2e$

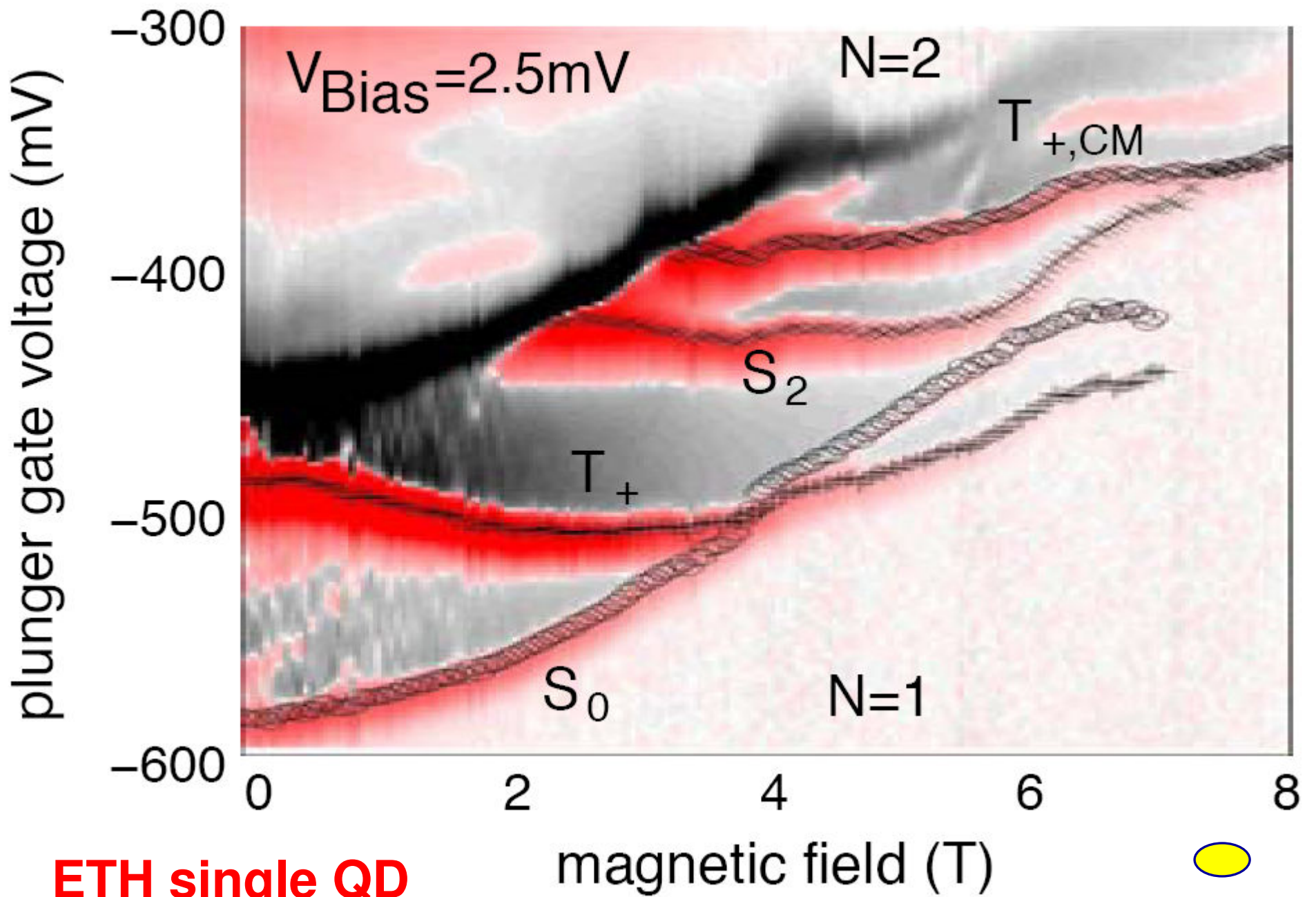


$\eta=0.72$

η =ratio of principal axes

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

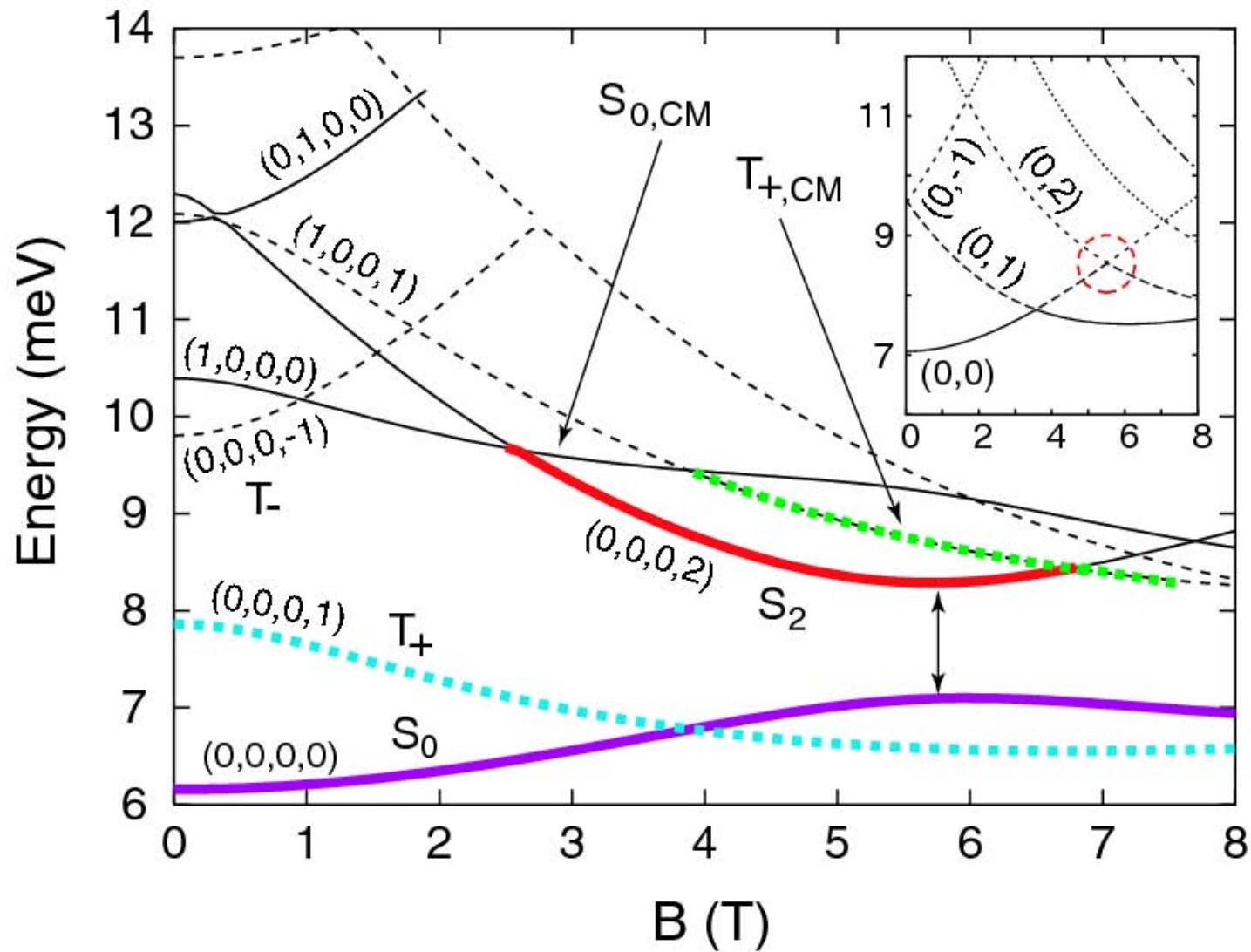




ETH single QD

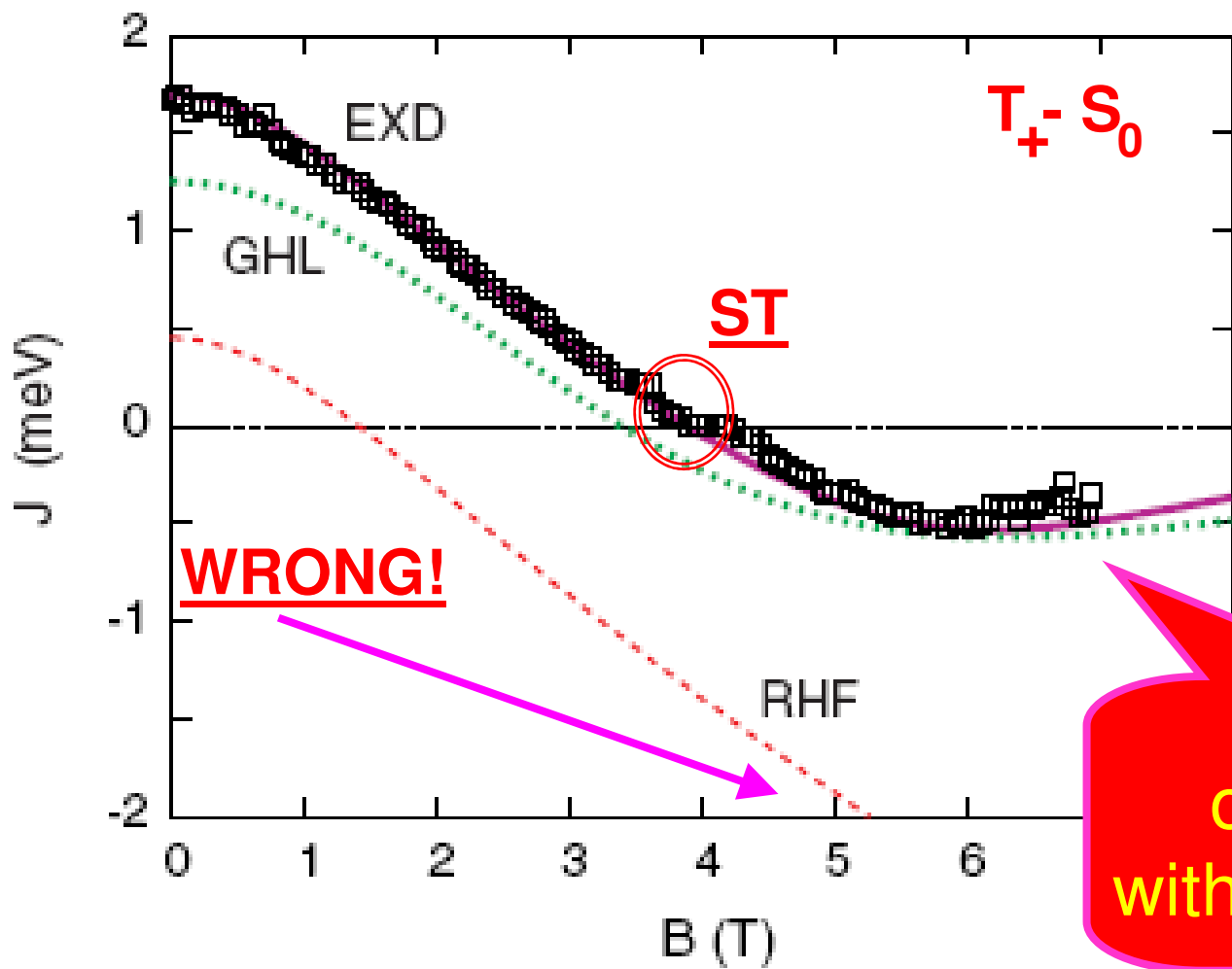
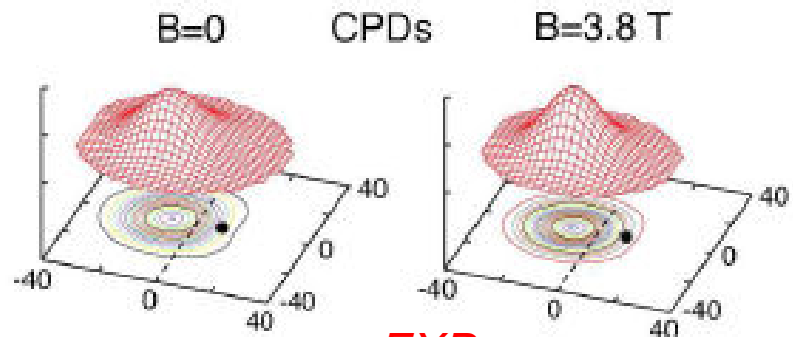
ETH single QD

EXD = Exact diagonalization



ETH single QD

$h\nu_x=4.23$ meV; $h\nu_y=5.84$ meV;
 $m^*=0.070$; $K=12.5$; $\gamma=0.86$



*Generalized
Heitler-London
wave function*

**Dissociation
of the 2e WM
within the single QD**

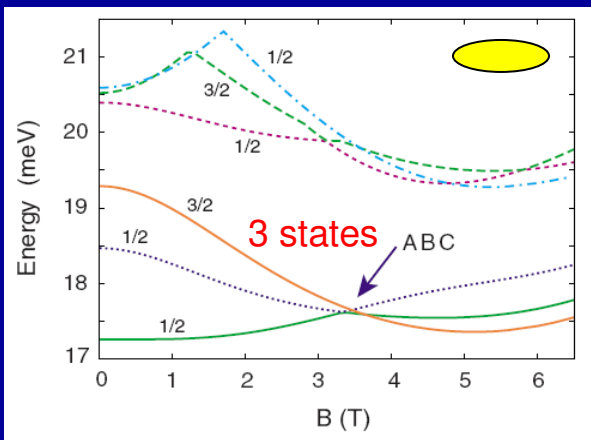
$N=3e$

Excitation spectra

Yuesong Li et al., PRB 76, 245310 (2007)

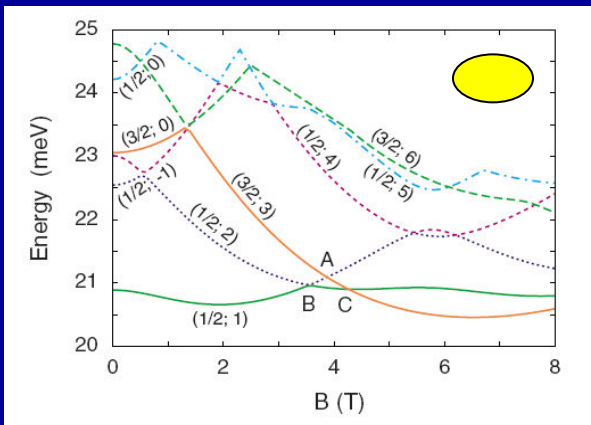
$\kappa=12.5$

$\eta=1/2$



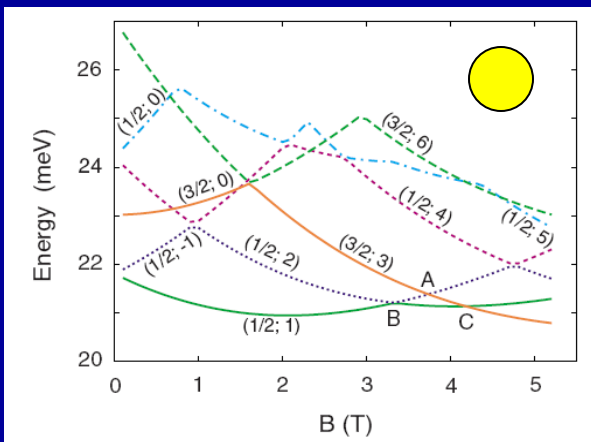
$\kappa=12.5$

$\eta=0.72$



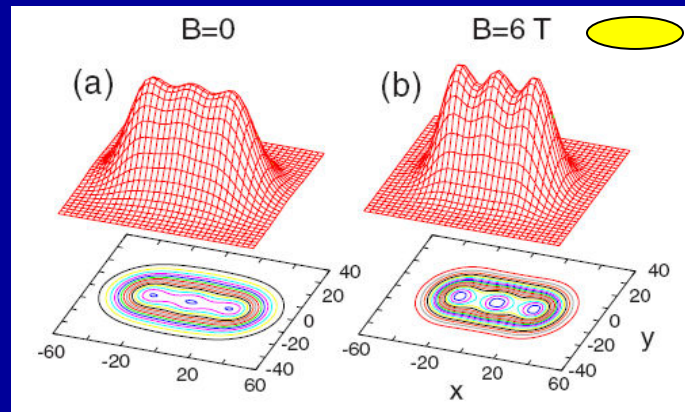
$\kappa=12.5$

$\eta=1$



$\kappa=12.5$

$\eta=1/2$



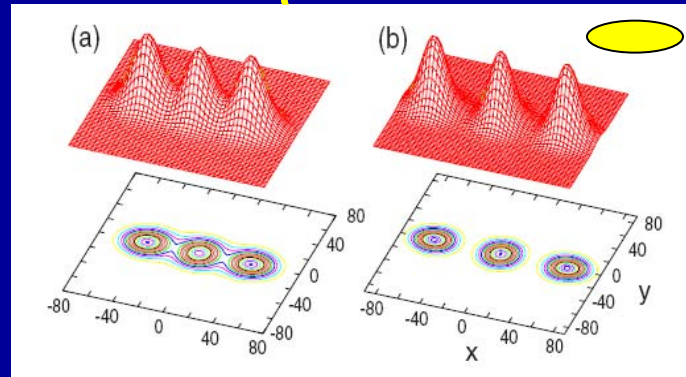
Electron densities

Pinned Wigner Molecule

$\kappa=3$

$\eta=1/2$

$\kappa=1$



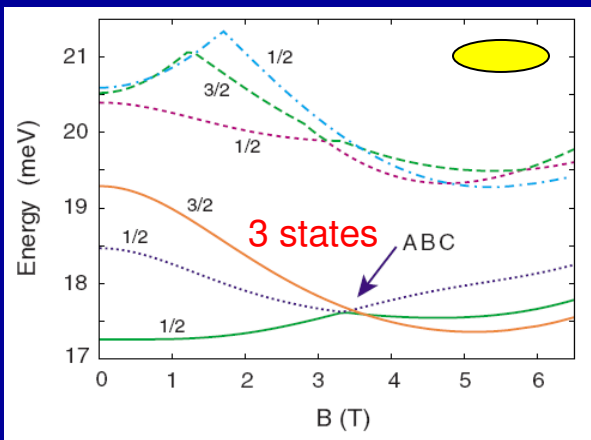
$N=3e$

Excitation spectra

Yuesong Li et al., PRB 76, 245310 (2007)

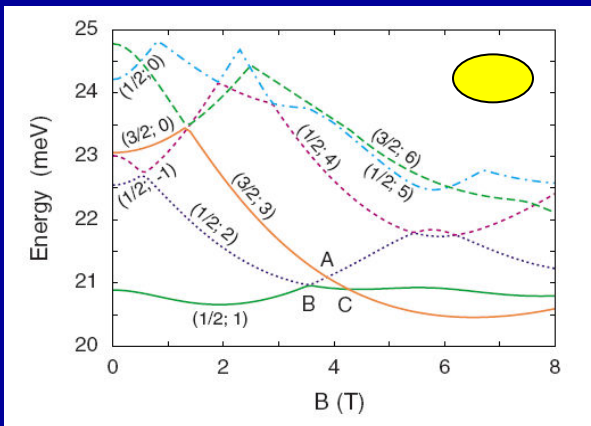
$\kappa=12.5$

$\eta=1/2$



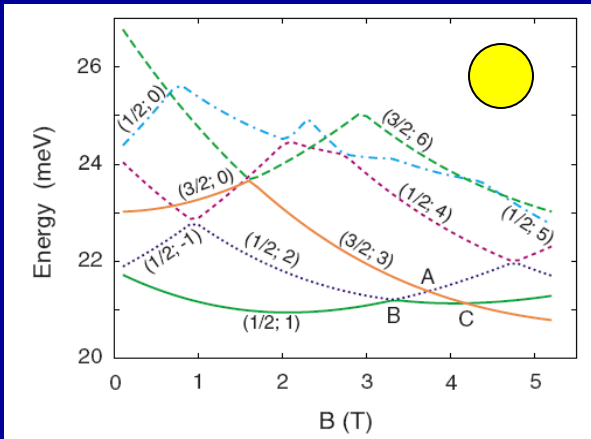
$\kappa=12.5$

$\eta=0.72$



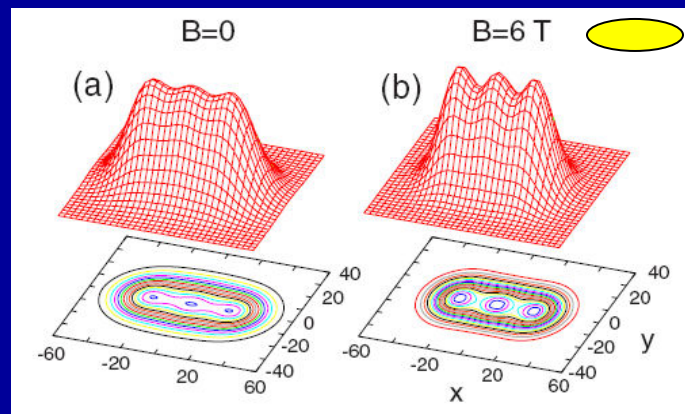
$\kappa=12.5$

$\eta=1$



$\kappa=12.5$

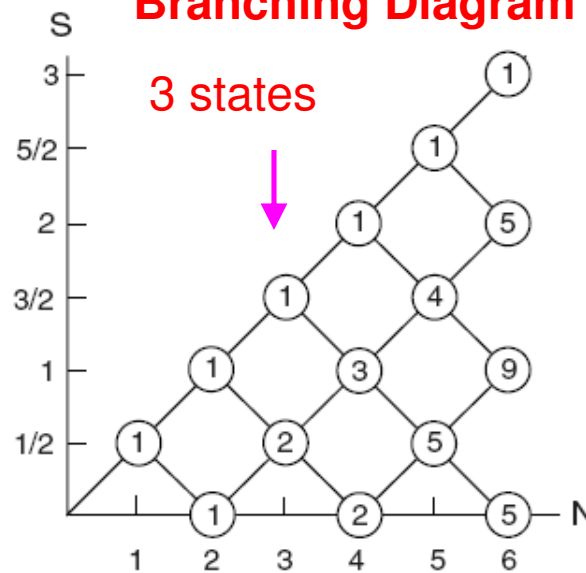
$\eta=1/2$



Electron densities

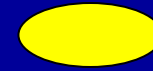
Branching Diagram

3 states



Formation of three-electron Wigner molecule

Elliptic QD



localized space orbitals



$$\alpha |\uparrow\downarrow\uparrow\rangle + \beta |\downarrow\uparrow\uparrow\rangle + \gamma |\uparrow\uparrow\downarrow\rangle$$

Entangled three-qubit W-states

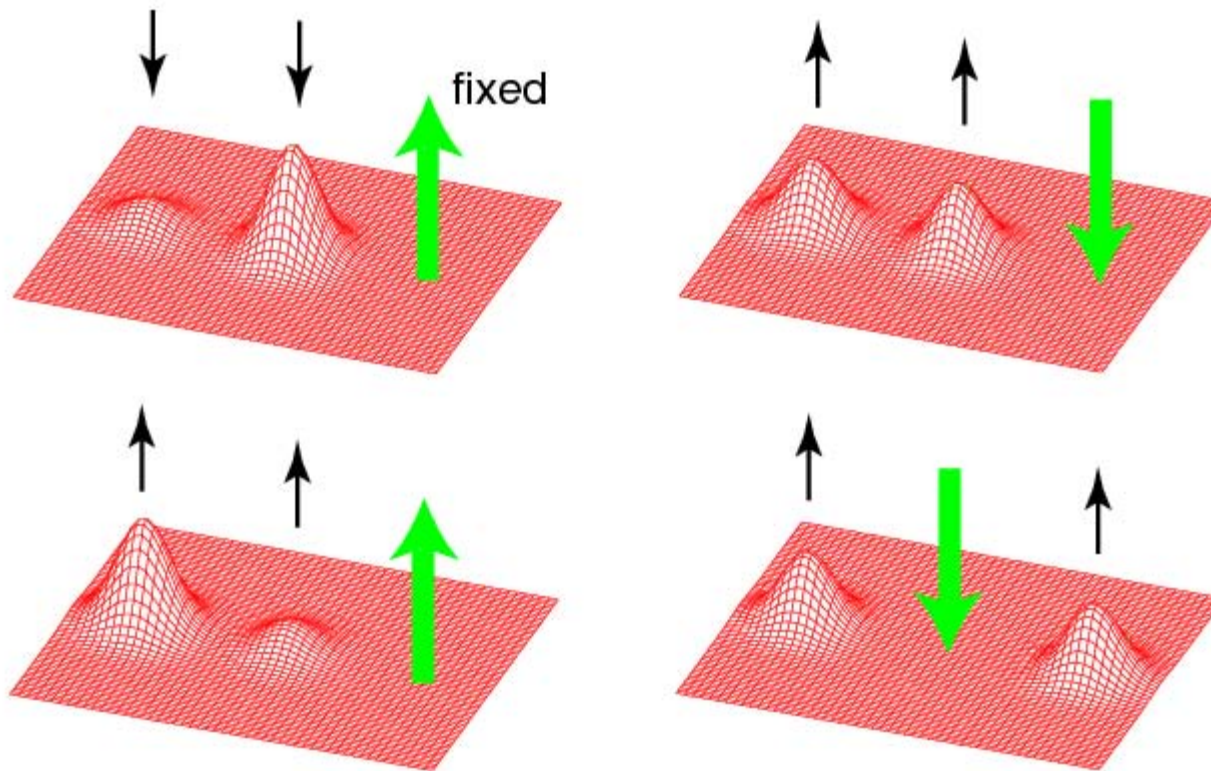
1) $\alpha=2, \beta=-1, \gamma=-1 \Rightarrow (1/2, 1/2; 1)$

2) $\alpha=0, \beta=1, \gamma=-1 \Rightarrow (1/2, 1/2; 2)$

3) $\alpha=\beta=\gamma=1 \Rightarrow (3/2, 1/2)$

Study entanglement by using
Spin resolved CPDs for EXD wfs

Ground-state $(1/2, 1/2)$; $\hbar\omega_x = 3.137$ meV; $\hbar\omega_x/\hbar\omega_y = 1/2$;
 $m^* = 0.067m_e$; $B=0$; $K=1$



EXD wf $\sim 2 | \uparrow \downarrow \uparrow \rangle - | \downarrow \uparrow \uparrow \rangle - | \uparrow \uparrow \downarrow \rangle$

Control and measurement of three-qubit entangled states

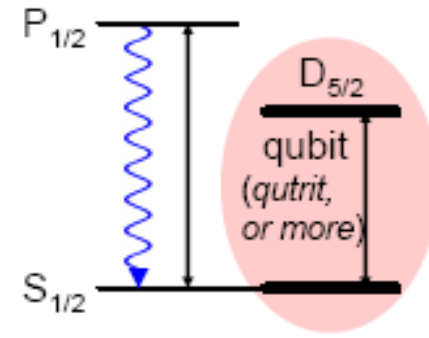
C. F. Roos¹, Mark Riebe¹, H. Häffner¹, W. Hänsel¹,
 J. Benhelm¹, G. P. T. Lancaster¹, C. Becher¹,
 F. Schmidt-Kaler¹ & R. Blatt^{1,2}

¹Institut für Experimentalphysik, Universität Innsbruck, Technikerstraße 25, A-6020 Innsbruck, Austria
²Institut für Quantenoptik und Quanteninformation, Österreichische Akademie der Wissenschaften

- Basics of ion trap quantum computers
- Entangling operations (Bell states, CNOT)
- Generation of W- and GHZ-states
- Selective read-out of a quantum register
- Entanglement transformation by conditional operations



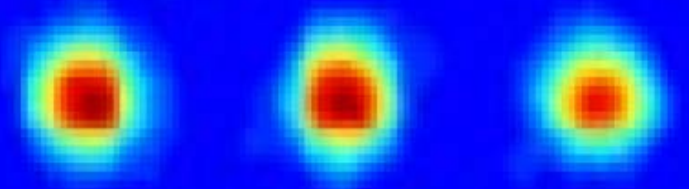
Qubits with trapped ions



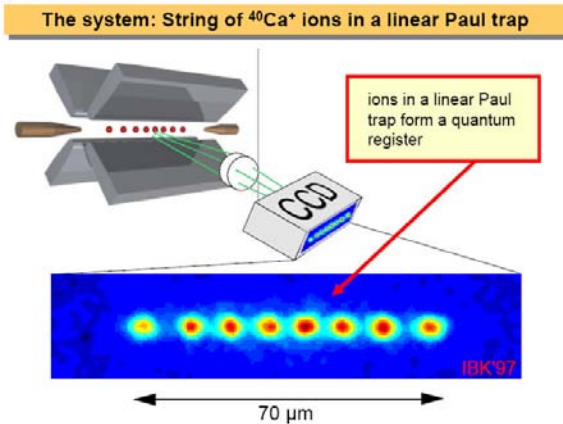
S – D transitions in alkaline earths:
 Ca^+ , Sr^+ , Ba^+ , Ra^+ , (Yb^+ , Hg^+) etc.

Entangled states with three ions

GHZ-states: $|SSS + DDD\rangle$



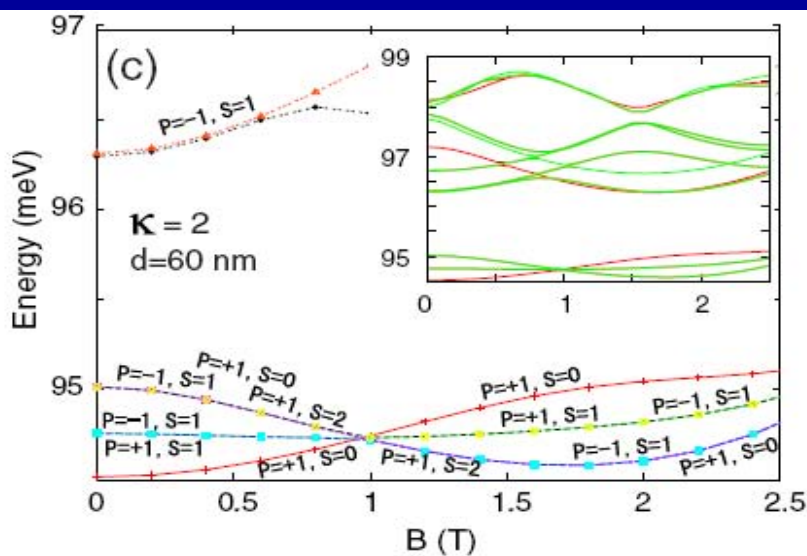
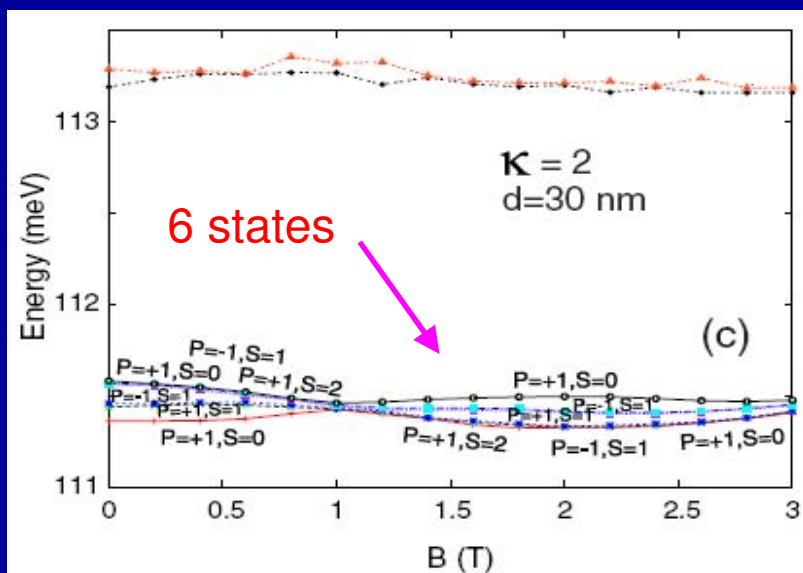
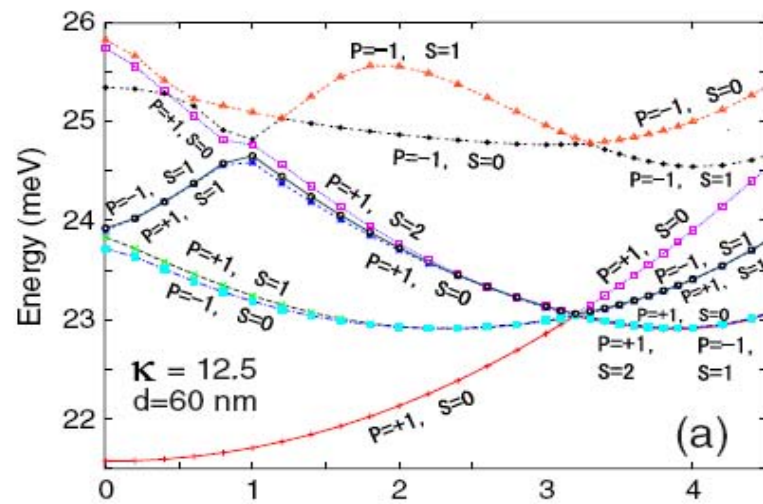
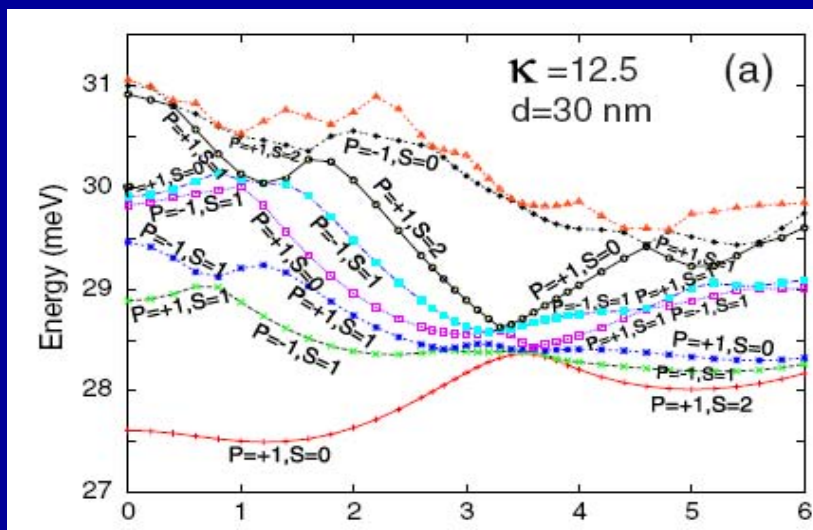
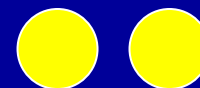
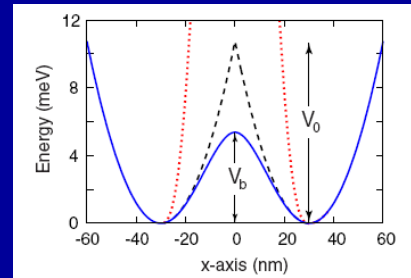
W-states: $|SDD + DSD + DDS\rangle$



Quantum Dot Helium Molecule

N=4e Ying Li et al.: PRB 80, 045326 (2009)

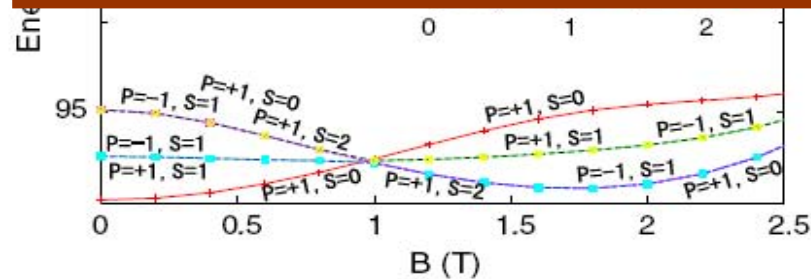
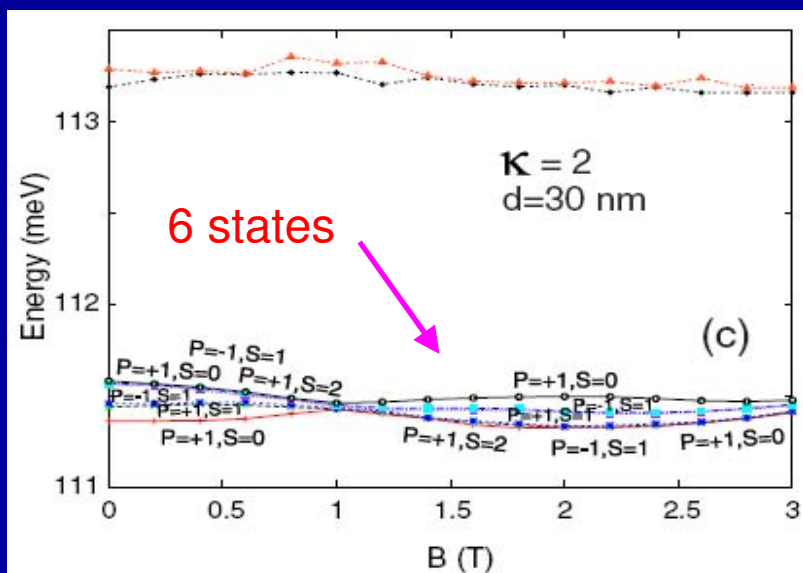
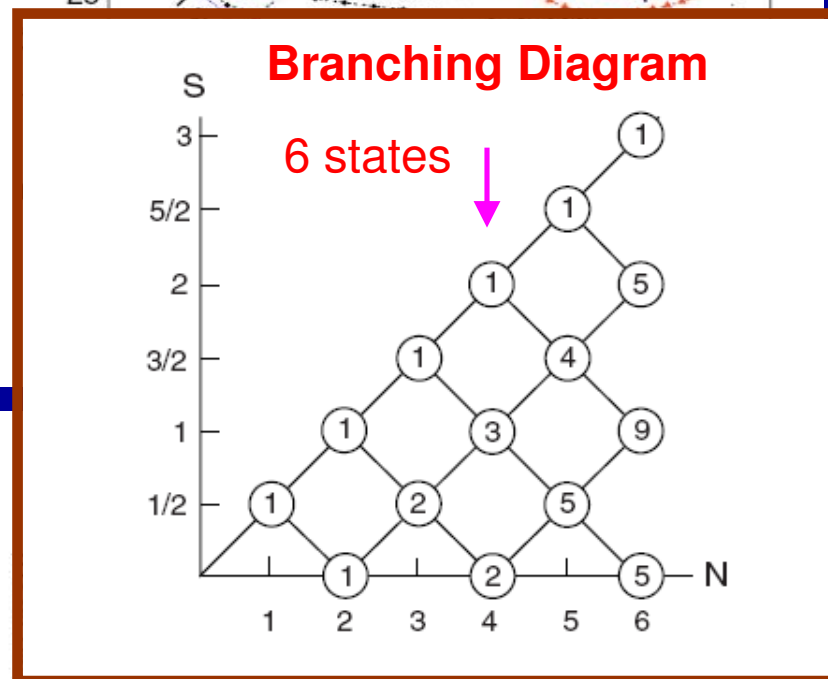
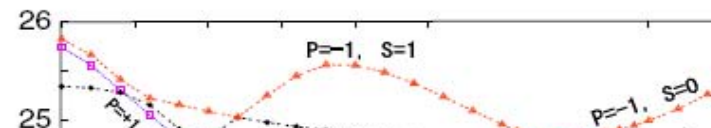
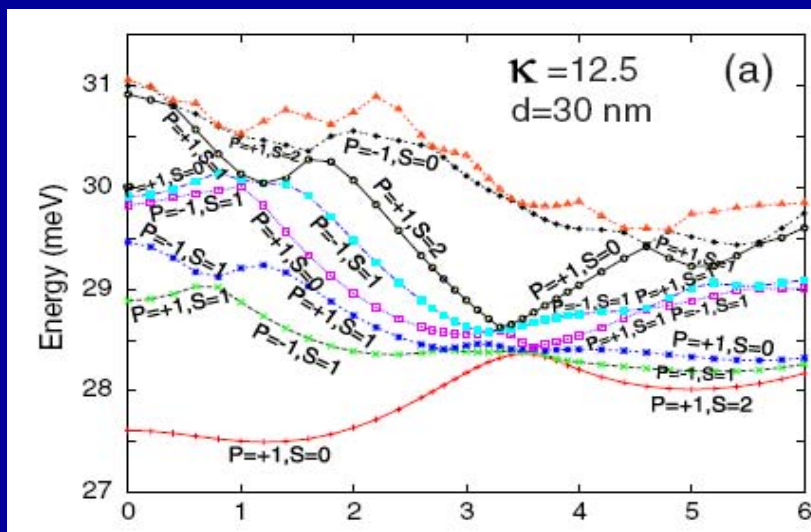
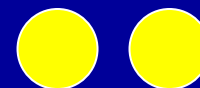
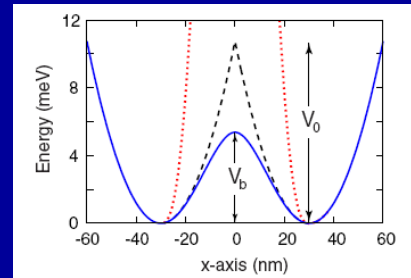
EXD calculation



Quantum Dot Helium Molecule

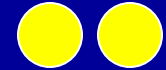
N=4e Ying Li et al.: PRB 80, 045326 (2009)

EXD calculation

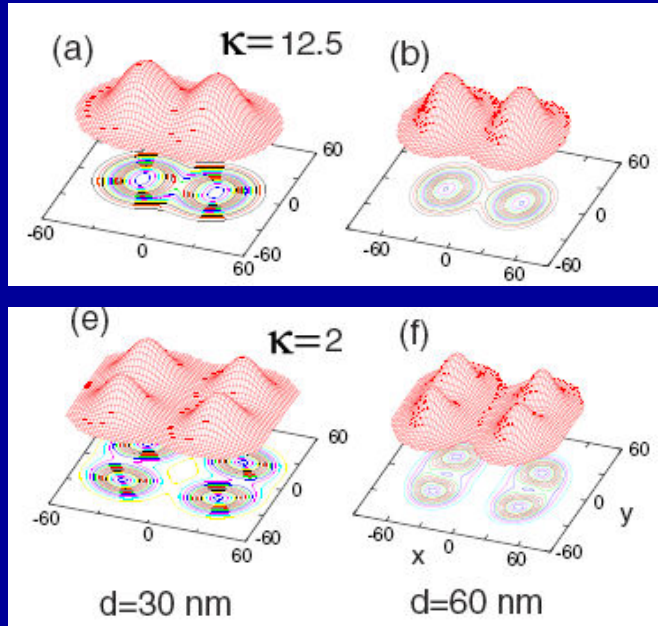


States at B=0

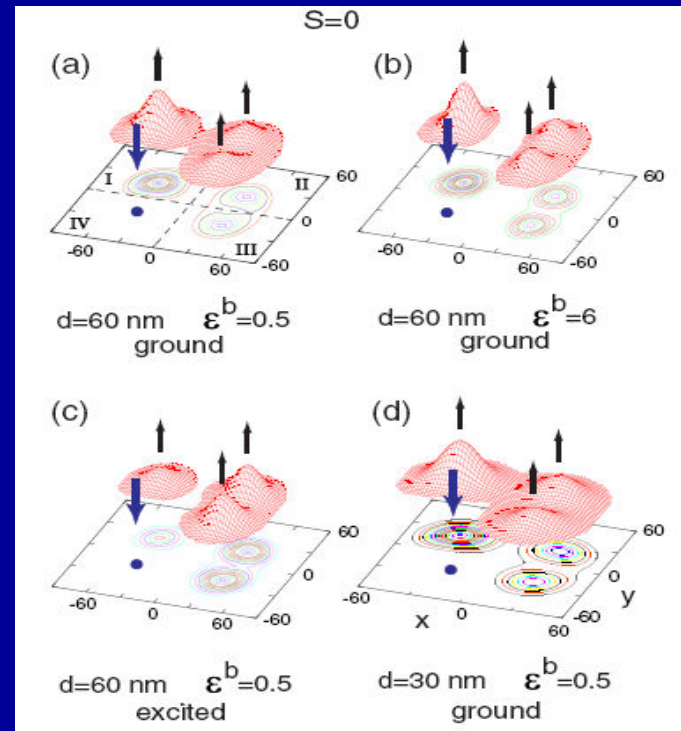
$$S = 0, S_z = 0$$



Ground State Electron Densities



Spin-resolved Pair Correlations



$\kappa=2$

$$|\Psi_N^{\text{EXD}}(S, S_z; k)\rangle = \sum_I C_I^N(S, S_z; k) |SD(I; N, S_z)\rangle$$



Spin functions

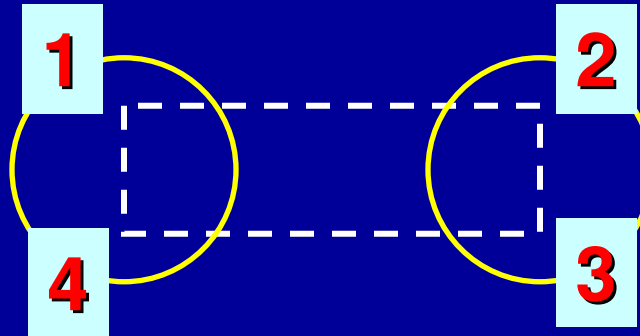
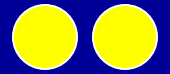
$I \sim 100,000$

Slater
Determinant

$$\mathcal{X}_{00}^{(1)} = -\frac{1}{2} |\uparrow\uparrow\downarrow\downarrow\rangle + \frac{1}{2} |\uparrow\downarrow\uparrow\downarrow\rangle + \frac{1}{2} |\downarrow\uparrow\downarrow\uparrow\rangle - \frac{1}{2} |\downarrow\downarrow\uparrow\uparrow\rangle$$

$$\mathcal{X}_{00}^{(2)} = \frac{1}{2\sqrt{3}} |\uparrow\uparrow\downarrow\downarrow\rangle + \frac{1}{2\sqrt{3}} |\uparrow\downarrow\uparrow\downarrow\rangle - \frac{1}{\sqrt{3}} |\uparrow\downarrow\downarrow\uparrow\rangle - \frac{1}{\sqrt{3}} |\downarrow\uparrow\uparrow\downarrow\rangle + \frac{1}{2\sqrt{3}} |\downarrow\uparrow\downarrow\uparrow\rangle + \frac{1}{2\sqrt{3}} |\downarrow\downarrow\uparrow\uparrow\rangle$$

4-site Heisenberg cluster



$$\mathcal{H}_H(B) = \tilde{J}_{12}(B)(\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_3 \cdot \mathbf{S}_4) + \tilde{J}_{14}(B)(\mathbf{S}_1 \cdot \mathbf{S}_4 + \mathbf{S}_2 \cdot \mathbf{S}_3)$$



$$S_z = 0$$

$$\frac{1}{2} \begin{pmatrix} \tilde{J}_{12} - \tilde{J}_{14} & \tilde{J}_{14} & 0 & 0 & \tilde{J}_{14} & 0 \\ \tilde{J}_{14} & -(\tilde{J}_{12} + \tilde{J}_{14}) & \tilde{J}_{12} & \tilde{J}_{12} & 0 & \tilde{J}_{14} \\ 0 & \tilde{J}_{12} & \tilde{J}_{14} - \tilde{J}_{12} & 0 & \tilde{J}_{12} & 0 \\ 0 & \tilde{J}_{12} & 0 & \tilde{J}_{14} - \tilde{J}_{12} & \tilde{J}_{12} & 0 \\ \tilde{J}_{14} & 0 & \tilde{J}_{12} & \tilde{J}_{12} & -(\tilde{J}_{12} + \tilde{J}_{14}) & \tilde{J}_{14} \\ 0 & \tilde{J}_{14} & 0 & 0 & \tilde{J}_{14} & \tilde{J}_{12} - \tilde{J}_{14} \end{pmatrix}$$

$$|1\rangle \rightarrow |\uparrow\uparrow\downarrow\downarrow\rangle \quad |2\rangle \rightarrow |\uparrow\downarrow\uparrow\downarrow\rangle \quad \dots \quad |6\rangle \rightarrow |\downarrow\downarrow\uparrow\uparrow\rangle$$

4-site Heisenberg cluster: energies and eigenvectors

$$\mathcal{E}_1 = -(\tilde{J}_{14} + \tilde{J}_{12})/2,$$

$$\mathcal{E}_2 = (\tilde{J}_{14} - \tilde{J}_{12})/2,$$

$$\mathcal{E}_3 = (\tilde{J}_{12} - \tilde{J}_{14})/2,$$

$$\mathcal{E}_4 = (\tilde{J}_{14} + \tilde{J}_{12})/2,$$

$$\mathcal{E}_5 = -(\tilde{J}_{14} + \tilde{J}_{12})/2 - Q(\tilde{J}_{14}, \tilde{J}_{12}),$$

$$\mathcal{E}_6 = -(\tilde{J}_{14} + \tilde{J}_{12})/2 + Q(\tilde{J}_{14}, \tilde{J}_{12}),$$

where

$$Q(a, b) = \sqrt{a^2 - ab + b^2}.$$

$$\mathcal{V}_1 = \{0, -1, 0, 0, 1, 0\}, \quad S = 1,$$

$$\mathcal{V}_2 = \{0, 0, -1, 1, 0, 0\}, \quad S = 1,$$

$$\mathcal{V}_3 = \{-1, 0, 0, 0, 0, 1\}, \quad S = 1,$$

$$\mathcal{V}_4 = \{1, 1, 1, 1, 1, 1\}, \quad S = 2,$$

$$\mathcal{V}_5 = \{1, -\mathcal{X}, -1 + \mathcal{X}, -1 + \mathcal{X}, -\mathcal{X}, 1\}, \quad S = 0,$$

$$\mathcal{V}_6 = \{1, -\mathcal{Y}, -1 + \mathcal{Y}, -1 + \mathcal{Y}, -\mathcal{Y}, 1\}, \quad S = 0,$$

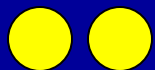
where

$$\mathcal{X} = r + Q(1, r),$$

$$\mathcal{Y} = r - Q(1, r),$$

and $r = \tilde{J}_{12}/\tilde{J}_{14}$.

Explain EXD spectra



Agree with EXD spin functions

$$\mathcal{V}_5 \rightarrow \{1, -1, 0, 0, -1, 1\}$$

$$\mathcal{V}_6 \rightarrow \{1, 1, -2, -2, 1, 1\}$$

SUMMARY

Under appropriate conditions, 2D electrons in anisotropic single and double quantum dots **do localize**, forming **pinned Wigner Molecules (PWMs)**

The **excitation spectra** and **spin functions** of PWMs can be understood via **finite-Heisenberg-cluster Hamiltonians** with B-dependent exchange constants $J(B)$.

Spin functions are associated with classes of well known strongly **entangled states**, e.g., W-states, Dicke states, etc...

Signatures of the Heisenberg-type spectra do survive even for weaker localization (corresponding to current available experimental lateral quantum dots).