NUCLEAR ASPECTS OF CONDENSED-MATTER NANOSYSTEMS

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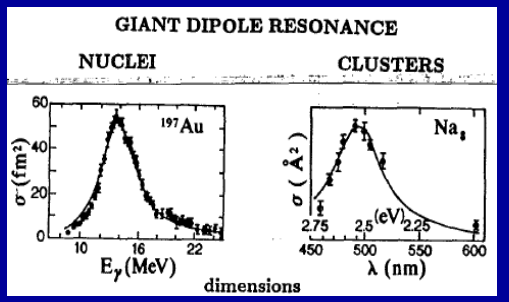
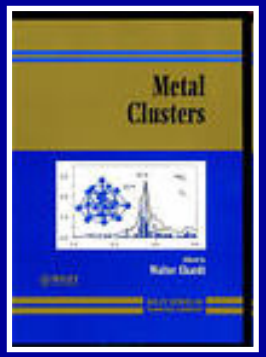
Three (among others) major nuclear aspects:

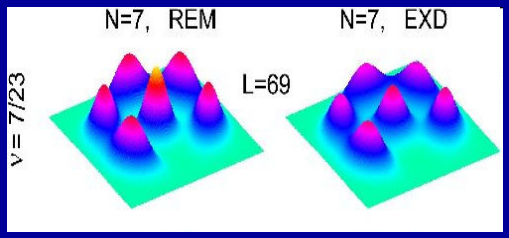
- *Surface plasmons/Giant resonances* (via matrix RPA/LDA) in metal clusters
  [see, e.g., Yannouleas, Broglia, Brack, Bortignon, PRL **63,** 255 (1989)]



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



- *Strongly correlated states (Wigner molecules)* 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)]



Strutinsky's approach and orbital-free density-functional methods for finite systems

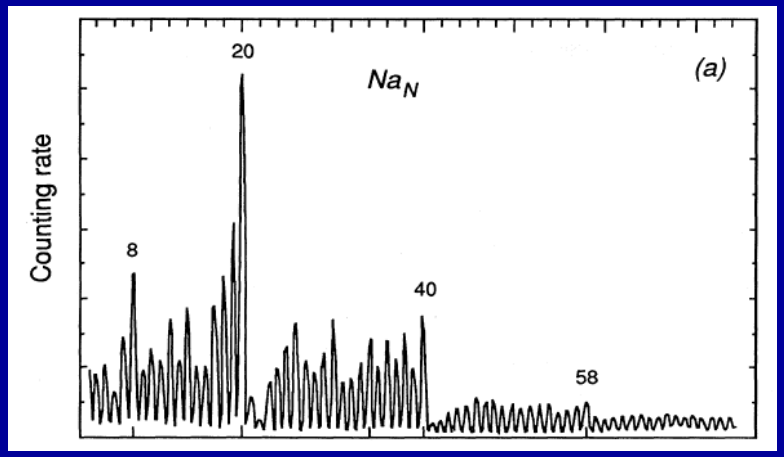
Invited talk at the *"Orbital-Free Density Functional Theory and Its Applications to Large-Scale Materials Simulations"*

Symposium at
"The 2010 International Chemical Congress of Pacific Basin Societies"

Strutinsky's approach → Shell correction method (SCM)

Electronic shells in 3D condensed-matter nanosystems:

(metal clusters, metallic nanowires, fullerenes, superatom-type systems: e.g., excited fullerenes, passivated gold clusters)



W.D. Knight et al., Phys. Rev. Lett. **52**, 2141 (1984)

8, 20, 40, 58, 92, 138, ...

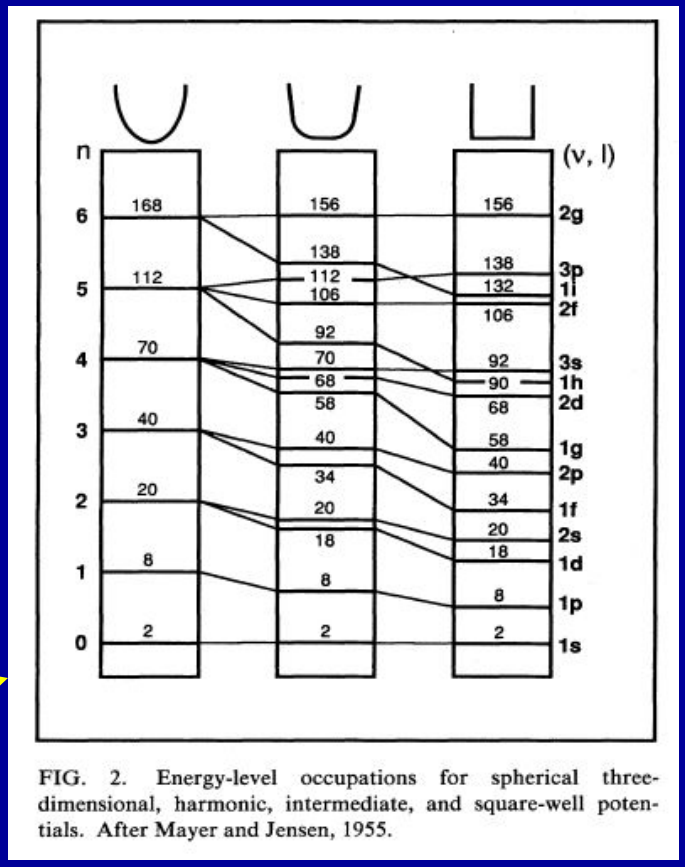
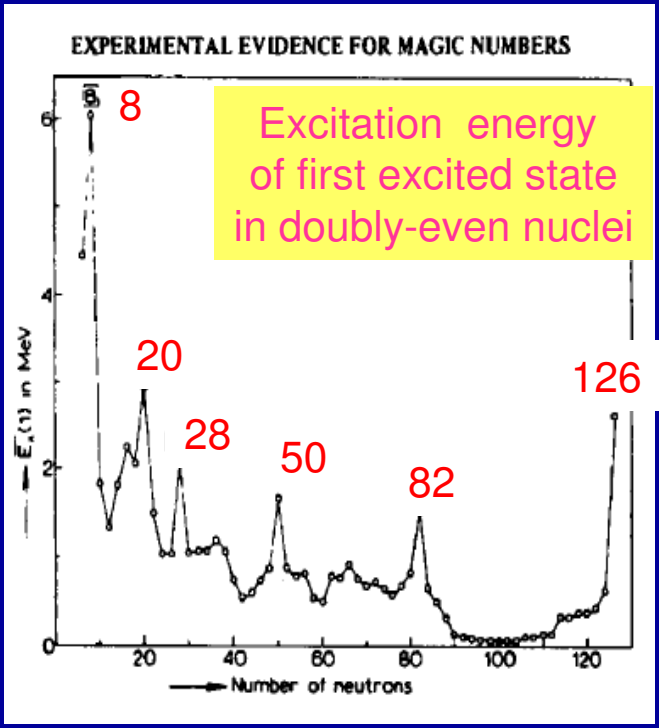


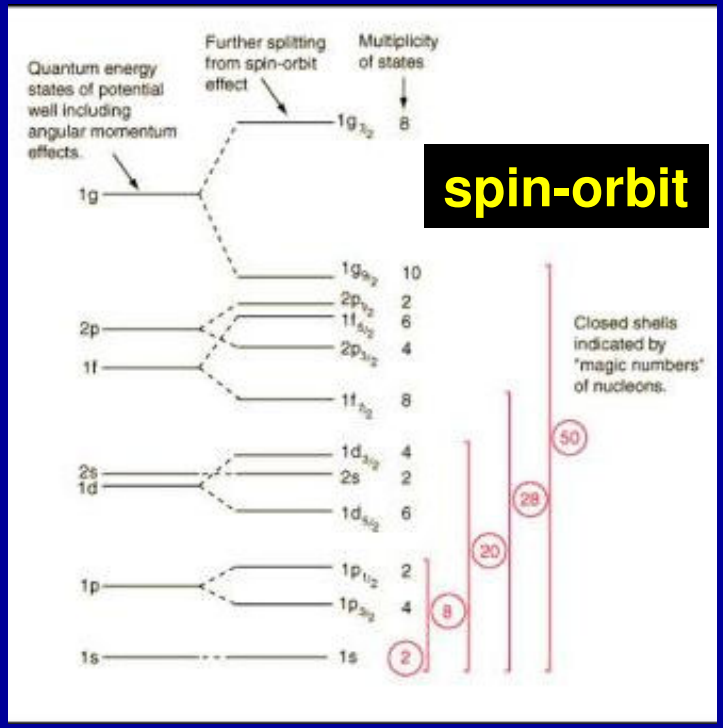
FIG. 2. Energy-level occupations for spherical three-dimensional, harmonic, intermediate, and square-well potentials. After Mayer and Jensen, 1955.

Qualitative explanation of magic numbers (most stable clusters): discrete single-particle energy levels in central potential

Nuclear Shell Model



Brussaard and Glaudemans 1977



Maria Goeppert Mayer
(1906-1972)

Hans Jensen
(1907-1973)

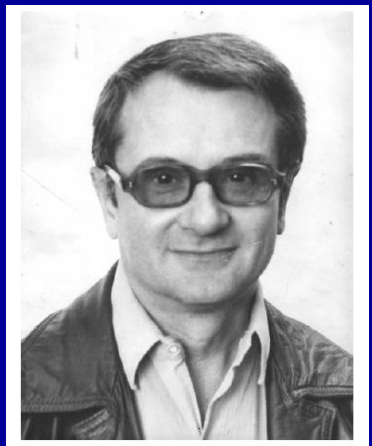
1963

Qualitative explanation of magic numbers (most stable nuclei):
Discrete single-particle energy levels in central potential

Quantitative theory: Strutinsky/Shell correction method in Nuclear Physics

V. M. Strutinsky, *Nucl. Phys. A* **95**, 420 (1967);
Nucl. Phys. A **122**, 1 (1968)

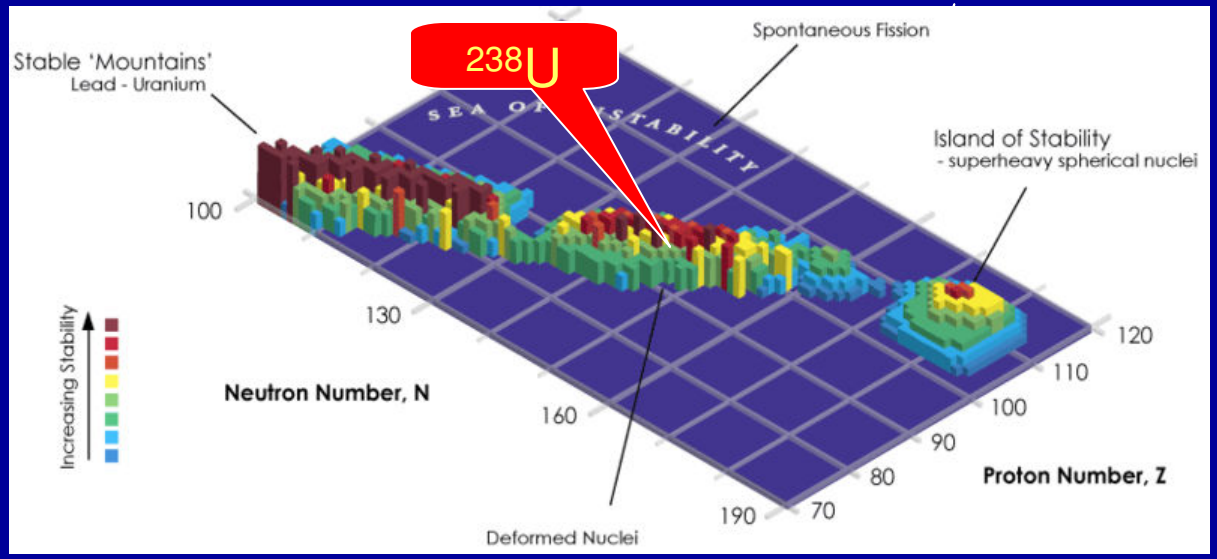
M. Brack et al., *Rev. Mod. Phys.* **44**, 320 (1972)


V.M. Strutinsky

V.M. Strutinsky

A famous prediction:

Super heavy nuclei: Island vs Peninsula of stability



TWO VARIANTS OF SCM in condensed-matter nanosystems:

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

Based on approximate sp density – Extended Thomas Fermi (ETF)

Literature: **Y&L,** PRB **48**, 8376 (1993) (condensed matter: metal clusters)

B. Zhou & Y.A. Wang, JCP **124**, 081107 2006; JCP **127**, 064101 (2007) (condensed matter: extended systems)

2) Semiempirical (SE-SCM)

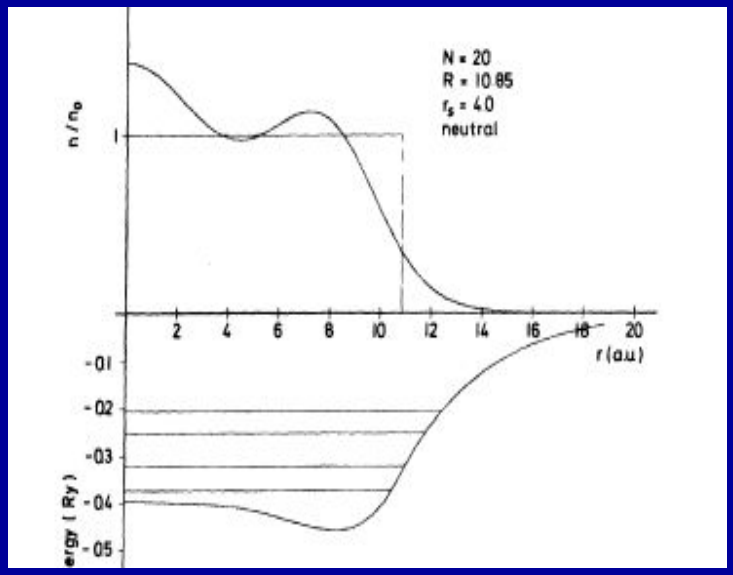
Based on an approximate central potential + liquid drop model for smooth variation

Y&L, PRB **51**, 1902 (1995) (condensed matter: metal clusters)

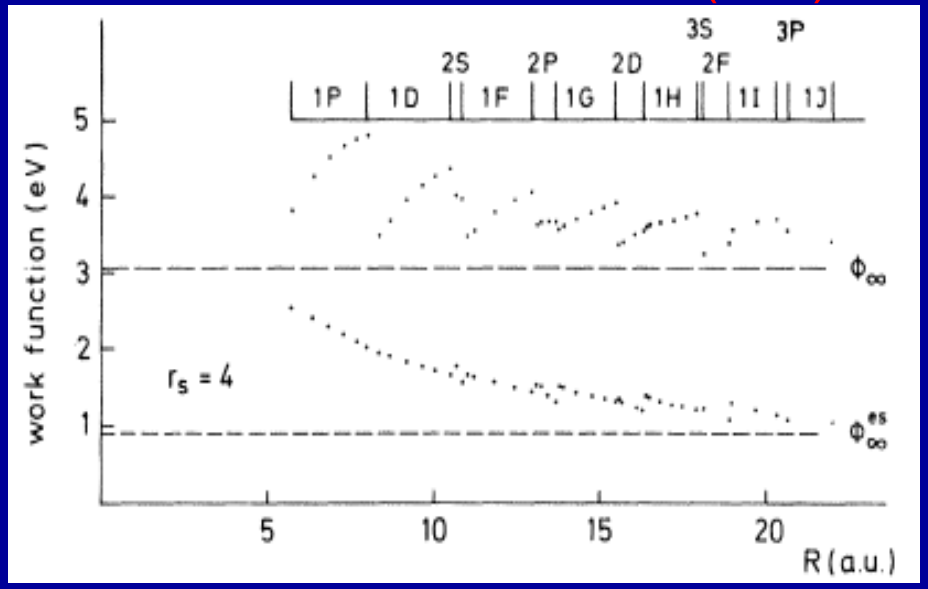
Used extensively in nuclear physics

DFT-SCM: Intuitive presentation

W. Ekardt, PRB **29**, 1558 (1984):
Na clusters, KS-DFT / 3D Spherical Jellium Background Model



Ionization Potentials (IPs)



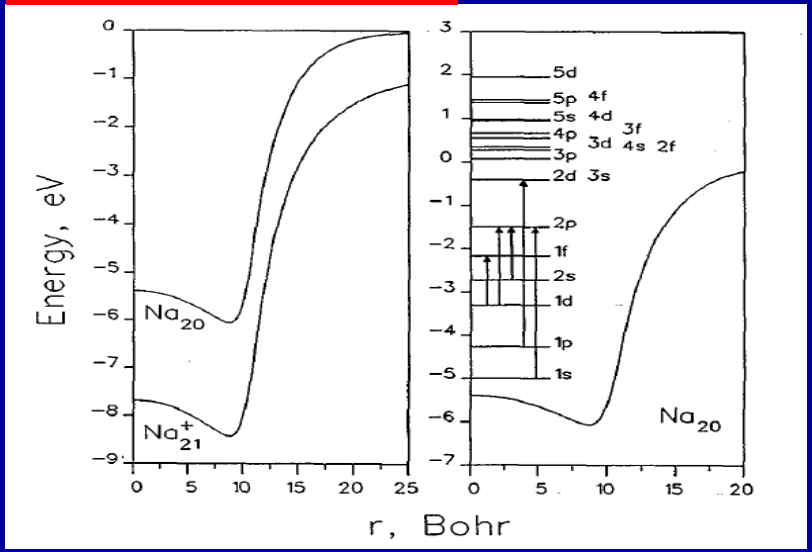
$$E_{\text{kin}} = \sum_{i=1}^{N} \langle i \mid -\Delta \mid i \rangle = \sum_{i=1}^{N} \epsilon_i - \int d\vec{r}\,\rho(\vec{r}) V(\vec{r};\rho(\vec{r}))$$

Kohn-Sham DFT

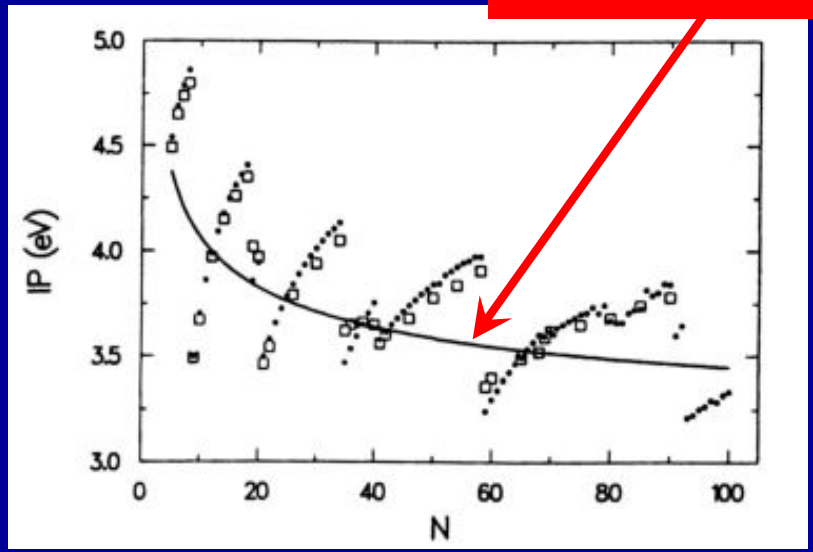
Shell effects derive from KEDF

What about the Extended Thomas Fermi (ETF)?

ETF potentials



ETF/ Smooth



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

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

Shell correction: Difference of two kinetic energy terms

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

Strutinsky's Theorem

$$\rho_{HF} = \widetilde{\rho} + \delta\rho$$

Self-consistent density = tilde smooth (ETF) + fluctuating parts

$$E_{HF} = \sum_{i=1}^{\text{occ}} \varepsilon_i^{HF} - \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\mathcal{V}(\mathbf{r}-\mathbf{r}')[\rho_{HF}(\mathbf{r},\mathbf{r})\rho_{HF}(\mathbf{r}',\mathbf{r}') - \rho_{HF}(\mathbf{r},\mathbf{r}')^2]$$

$$E_{Str} = \sum_{i=1}^{\text{occ}} \widetilde{\varepsilon}_i - \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\mathcal{V}(\mathbf{r}-\mathbf{r}')[\widetilde{\rho}(\mathbf{r},\mathbf{r})\widetilde{\rho}(\mathbf{r}',\mathbf{r}') - \widetilde{\rho}(\mathbf{r},\mathbf{r}')^2]$$

$$E_{HF} = E_{Str} + O(\delta\rho^2)$$

Self-consistent KS-DFT

$$T[\rho_{KS}] = \sum_{i=1}^{\text{occ}} \varepsilon_{KS,i} - \int \rho_{KS}(\mathbf{r}) V_{KS}[\rho_{KS}(\mathbf{r})] d\mathbf{r}$$

KEDF

$$E[\rho] = T[\rho] + \int \left\{ \left[\frac{1}{2} V_H[\rho(\mathbf{r})] + V_I(\mathbf{r}) \right] \rho(\mathbf{r}) \right\} d\mathbf{r} + \int \mathcal{E}_{xc}[\rho(\mathbf{r})] d\mathbf{r} + E_I$$

$$T_{ETF}[\rho] = \frac{\hbar^2}{2m} \int \left\{ \frac{3}{5}(3\pi^2)^{2/3} \rho^{5/3} + \frac{1}{36} \frac{(\nabla\rho)^2}{\rho} + \frac{1}{270}(3\pi^2)^{-2/3} \rho^{1/3} \times \left[\frac{1}{3} \left(\frac{\nabla\rho}{\rho} \right)^4 - \frac{9}{8} \left(\frac{\nabla\rho}{\rho} \right)^2 \frac{\Delta\rho}{\rho} + \left(\frac{\Delta\rho}{\rho} \right)^2 \right] \right\} d\mathbf{r},$$

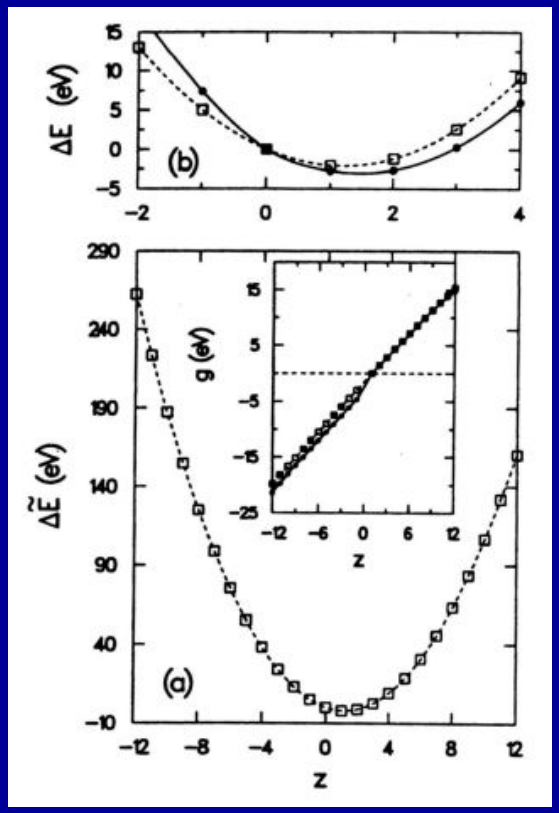
4th order

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

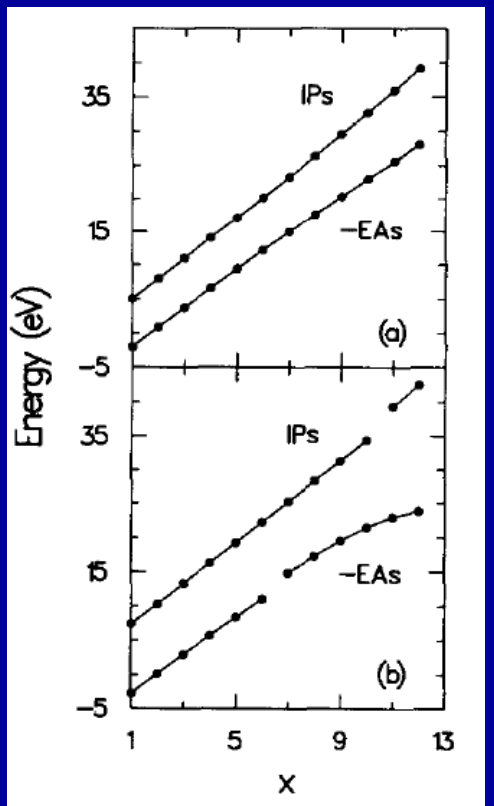
Non-self-consistent (orbital-free) DFT-SCM

Applications of DFT-SCM: multiply charged fullerene C_{60}

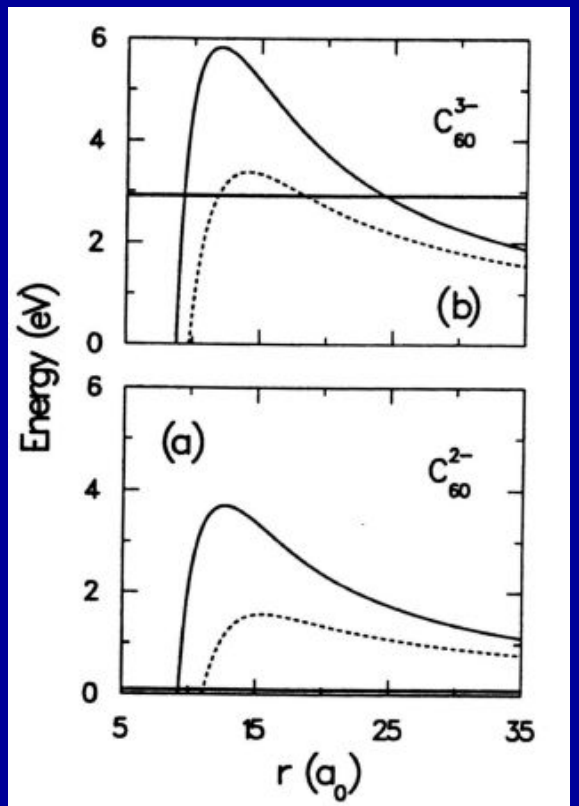
Y&L, Chem. Phys. Lett. **217**, 175 (1994)



Charging energies
(Capacitor)



Ionization
Potentials/
Electron
Affinities



RCB
Electron autodetachement

DFT-SCM: Shell correction

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

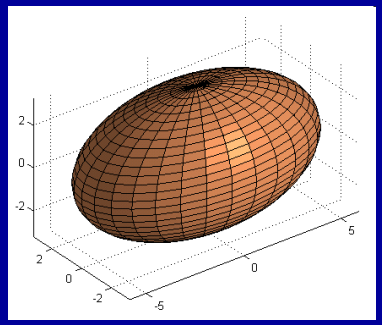
SE-SCM: Shell correction

$$\Delta E_{sh}^{Str} = \sum_{i=1}^{\text{occ}} \widetilde{\varepsilon}_i - \widetilde{E}_{sp}$$

$$\widetilde{E}_{sp} = \sum_{i} \widetilde{\varepsilon}_i \widetilde{f}_i.$$

$$H_0 = -\frac{\hbar^2}{2m_e} \triangle + \frac{m_e}{2}(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2)$$

$$H_N = H_0 + U_0 \hbar\omega_0 (\mathbf{l}^2 - < \mathbf{l}^2 >_n),$$

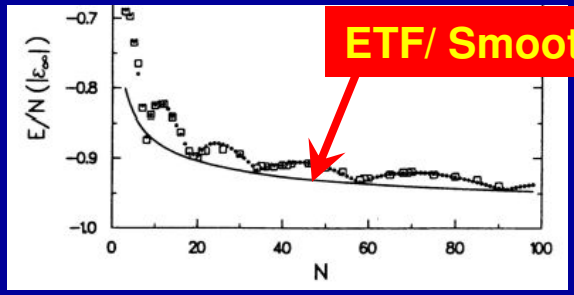


Y&L, PRB **51,** 1902 (1995)

Modified Nilsson potential
(triaxial oscillator)

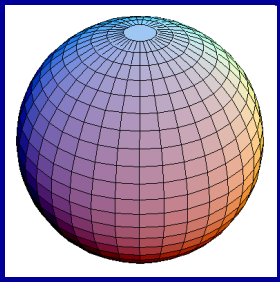
SE-SCM: Liquid drop model (LDM) component

ETF (smooth) energy: expansion in N, $N^{2/3}$, $N^{1/3}$)



volume surface curvature

$$E_{ETF}^{sph} = \alpha_v N + \alpha_s N^{2/3} + \alpha_c N^{1/3}$$



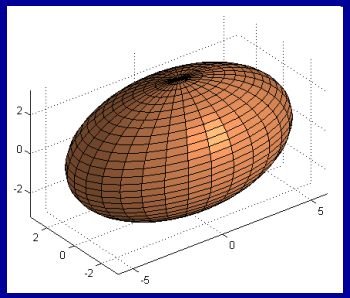
charging

$$\Delta\widetilde{E}^{sph}(Z) = \widetilde{E}^{sph}(Z) - \widetilde{E}^{sph}(0) = \mp WZ + \frac{Z(Z \pm 0.25)e^2}{2(R_0 + \delta)},$$

Capacitor

surface

$$\frac{E_{surf}^{ell}}{E_{surf}^{sph}} = \frac{ab}{2}\left[\frac{1 - e_1^2}{e_1}\mathcal{F}(\psi, k_3) + e_1\mathcal{E}(\psi, k_3) + c^3\right]$$



charging

$$\frac{\Delta\widetilde{E}^{ell}(Z) \pm WZ}{\Delta\widetilde{E}^{sph}(Z) \pm WZ} = \frac{bc}{e_1}\mathcal{F}(\psi, k_2),$$

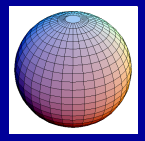
Y&L, PRB **51,** 1902 (1995)

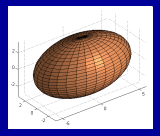
Examples of quantitative description with SE-SCM:
Ionization potentials

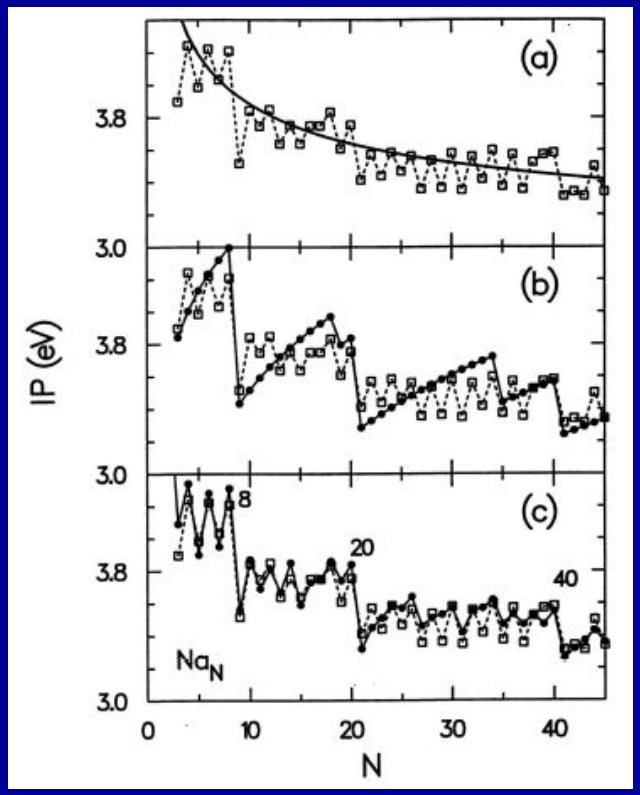
Sodium clusters/ zero temperature

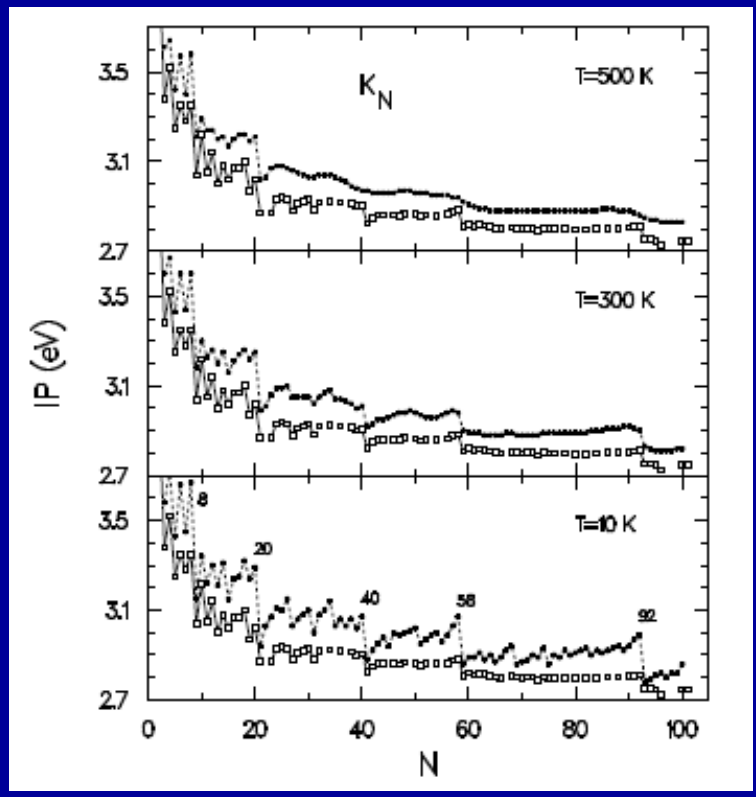
Potassium clusters/ temperature

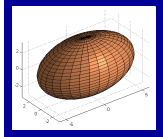
Smooth/
ETF

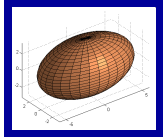


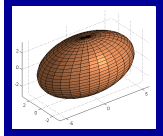












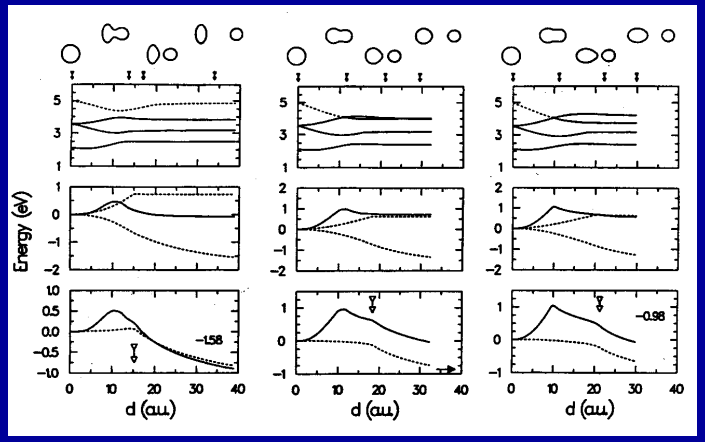
odd-even oscillations

Y&L, PRB **51,** 1902 (1995)

Y&L, PRL **78,** 1424 (1997)

$2\pi^2 T/(\hbar\omega_{\mathrm{sh}})$

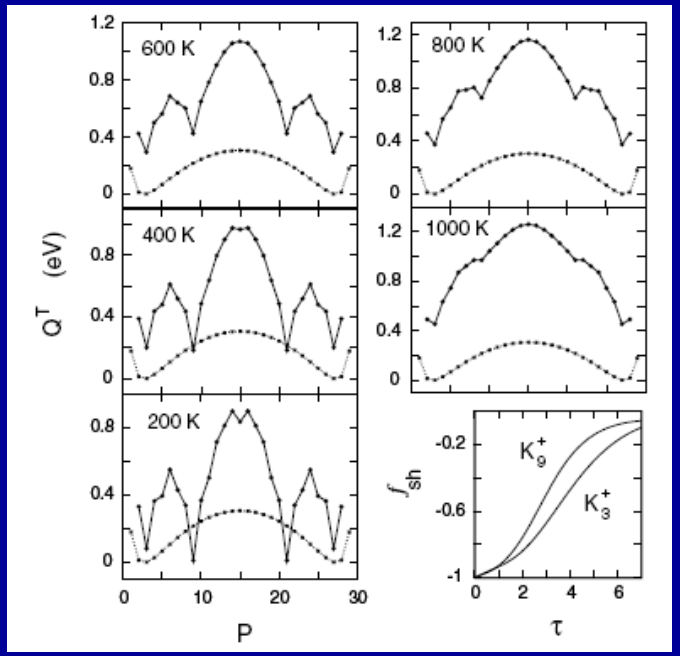
Electronic shells and fission of charged 3D Metal Clusters



Fission barriers/
Two-center oscillator potential model

$$Na_{10}^{2+} \rightarrow Na_7^{+} + Na_3^{+}$$

Yannouleas and Landman,
J. Phys. Chem. 99, 14577 (1995)



TEMPERATURE EFFECTS

Thermal quenching of electronic shells in cluster fission

$$K_{30}^{2+} \rightarrow K_P^{+} + K_{30-P}^{+}$$

C. Yannouleas, U. Landman, C. Brechignac, Ph. Cahuzac, B. Concina, and J. Leygnier , Phys. Rev. Lett. **89,** 173403 (2002)

SUMMARY (Shell Correction Method)

Shell Correction Method provides a quantitatively accurate approach for calculating the effects from the KEDF term (electronic shell effects) in *finite* condensed-matter systems

Two variants: OF-DFT-SCM (employing ETF/ 4^{th}-order?)
Semiempirical-SCM (external potential +LDM)

SCM can be generalized to *extended* systems
(work by Y.A. Wang and coworkers)

An unexpected journey: from nuclear physics (Strutinsky 1967)
to metal clusters (1993)
to orbital-free-DFT for extended systems (2006)

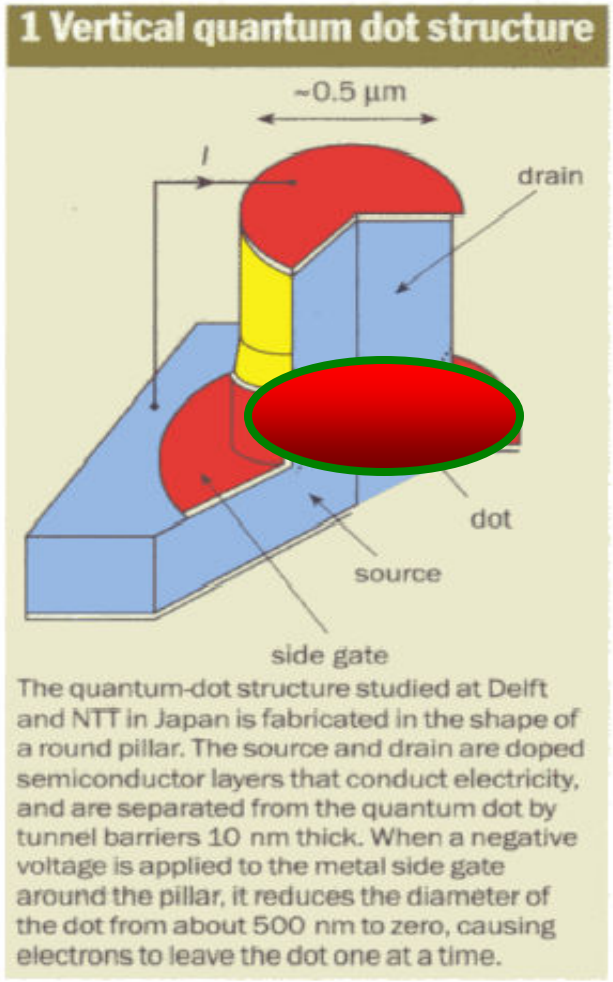
SECOND PART

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

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

Collaborators:

Igor Romanovsky (ultracold bosons & graphene dots)
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

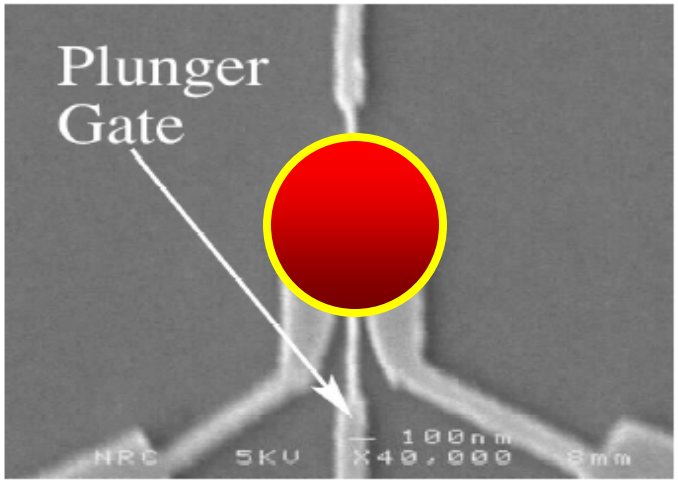
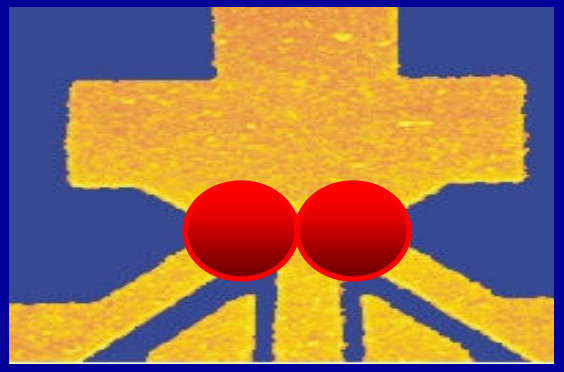


FIG. 1. SEM image of the gate geometry forming the quantum dot. This geometry enables a precisely known number of electrons ($N=0,1,2,\ldots,50$) to be trapped (Ref. 13) and produces a quasiparabolic confinement potential. Sweeping the plunger-gate voltage tunes both the shape and the chemical potential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

Lateral QD (Ottawa)

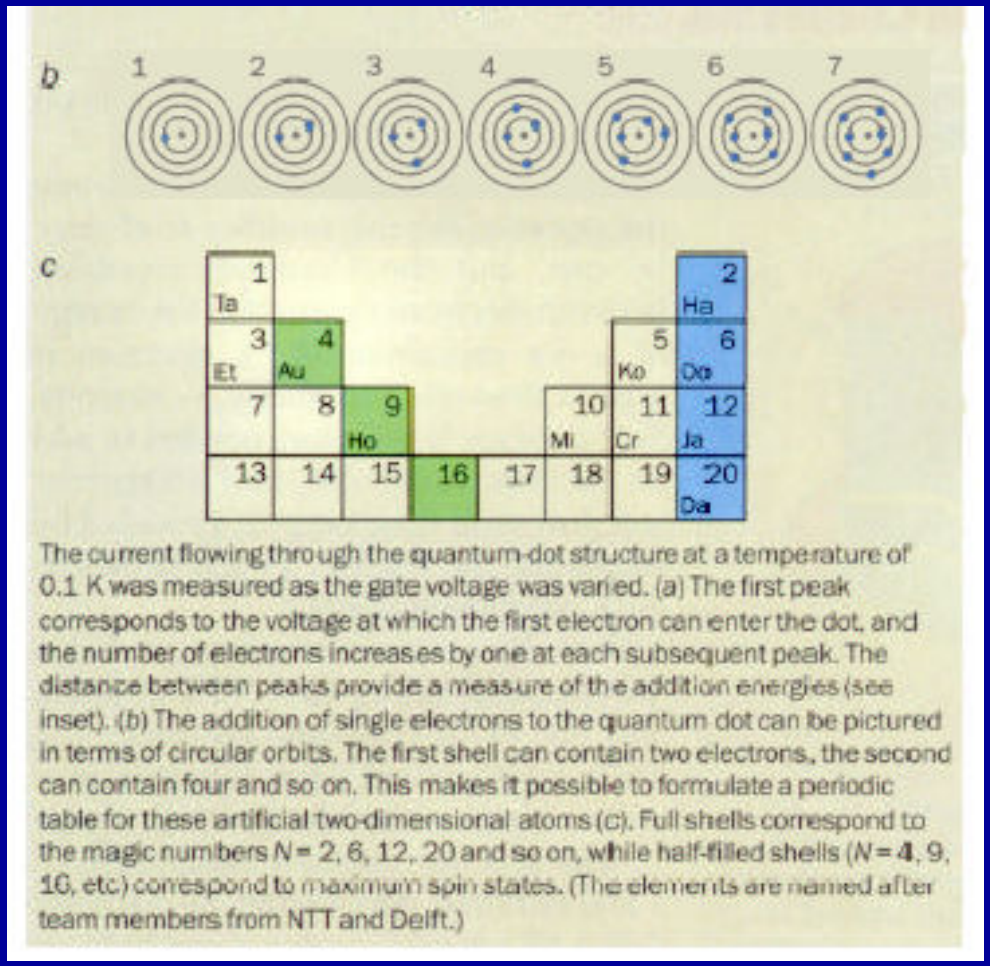


Lateral QD Molecule (Delft)

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

Nobel prize 1963

with Goeppert-Mayer/ Jensen

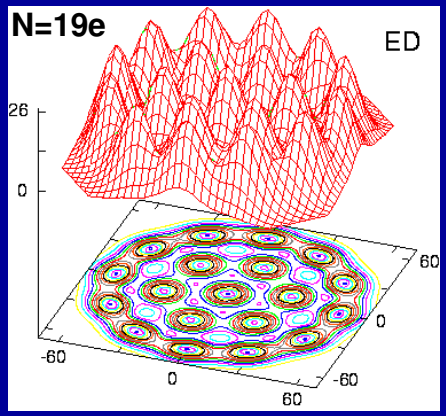
… electrons repell each other and try to keep as far apart as possible. The total energy of the system will be decreased through the corresponding modification of the wave function.
… "correlation energy" …

"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 … "

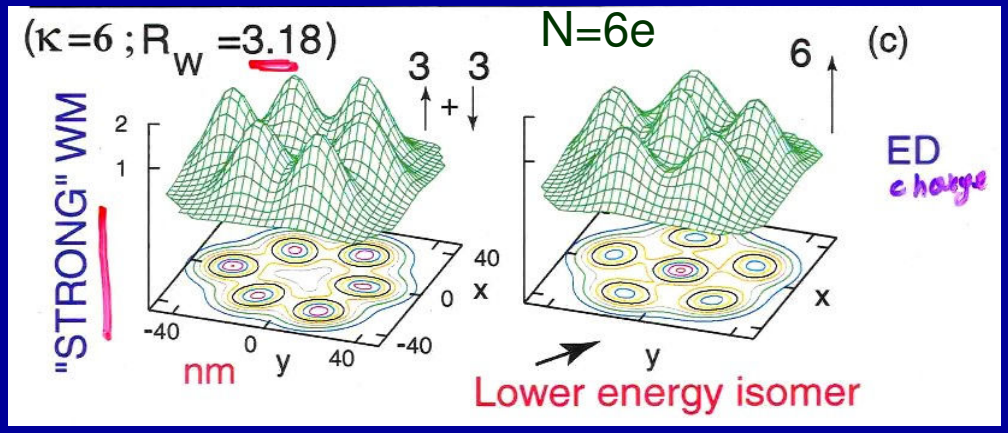
not for Wigner crystal

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)

Coulomb ➡ No capacitor

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

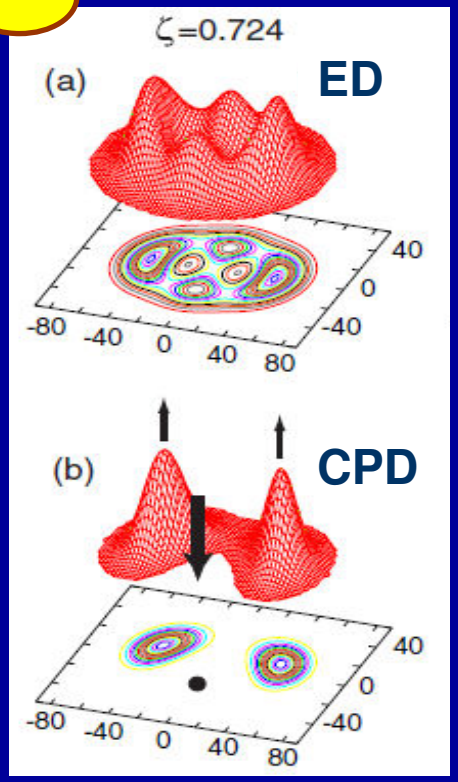
Three electron anisotropic QD

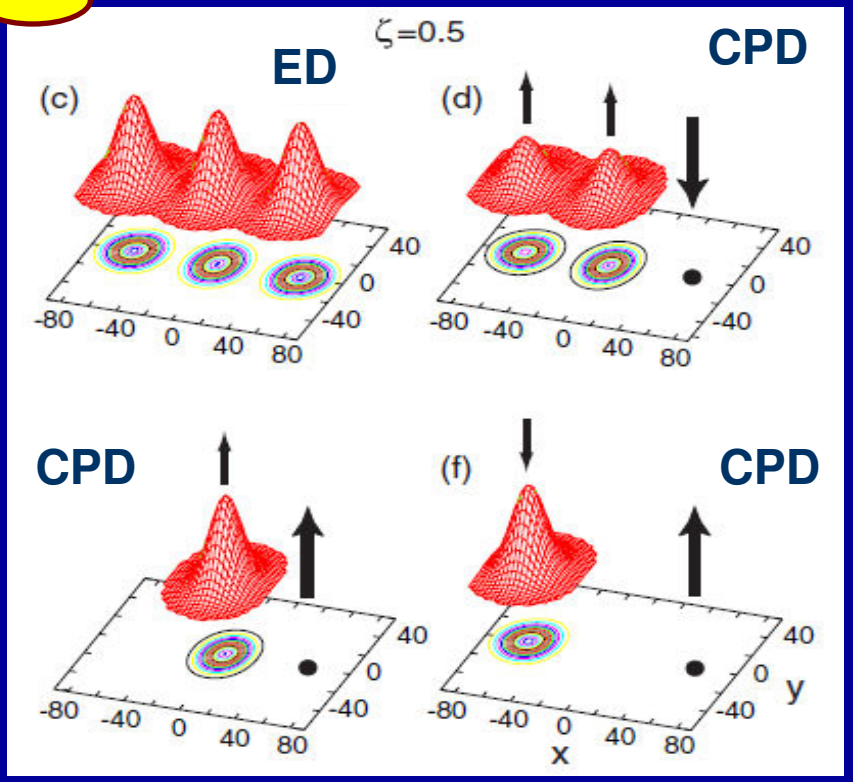
Method: ***Exact Diagonalization (EXD)***

Anisotropic confinement

Electron Density (ED)

(spin resolved) Conditional Probability Distribution (CPD)





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

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

Entangled three-qubit W-states

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

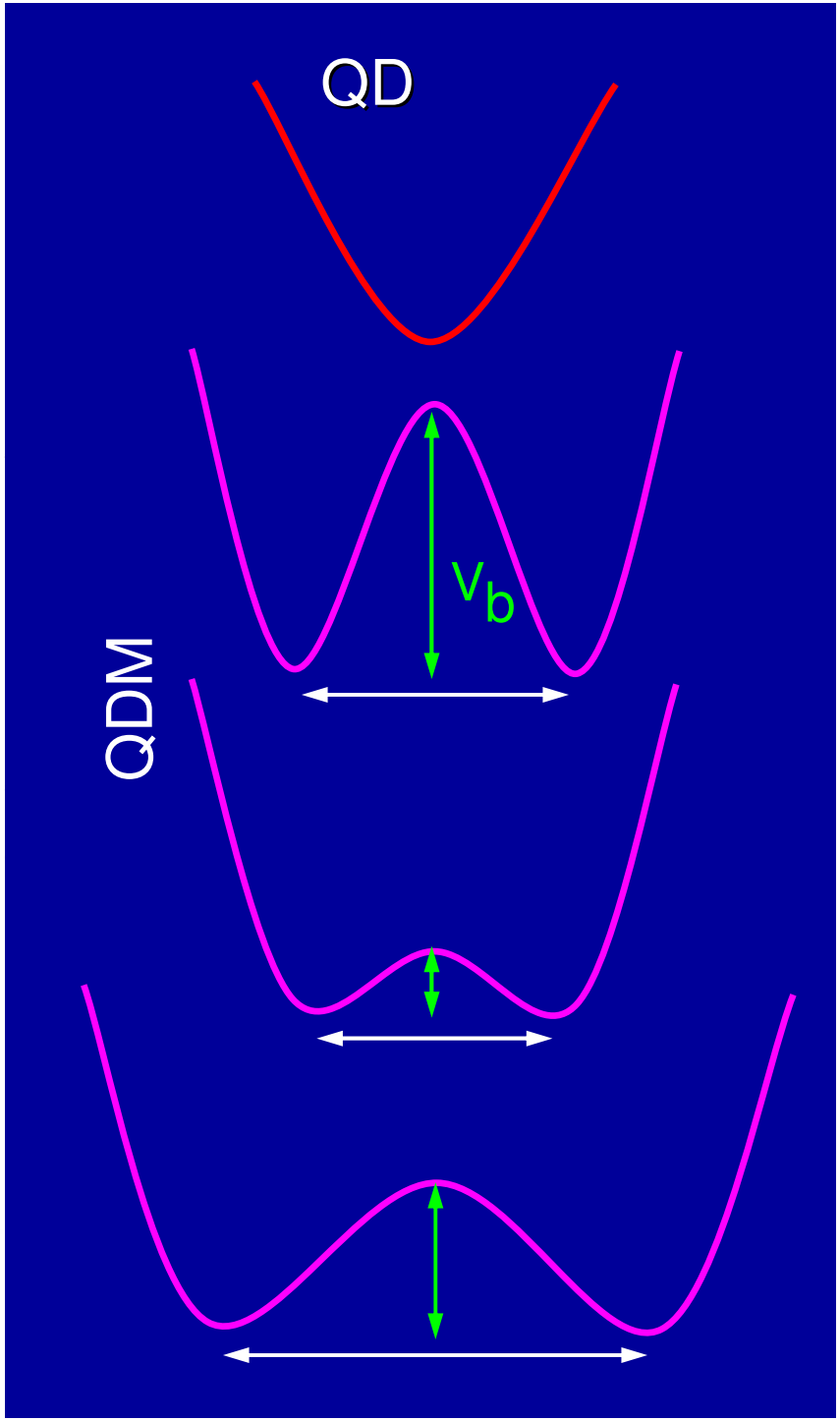
Two-center oscillator with V_b control } QDM

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

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

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

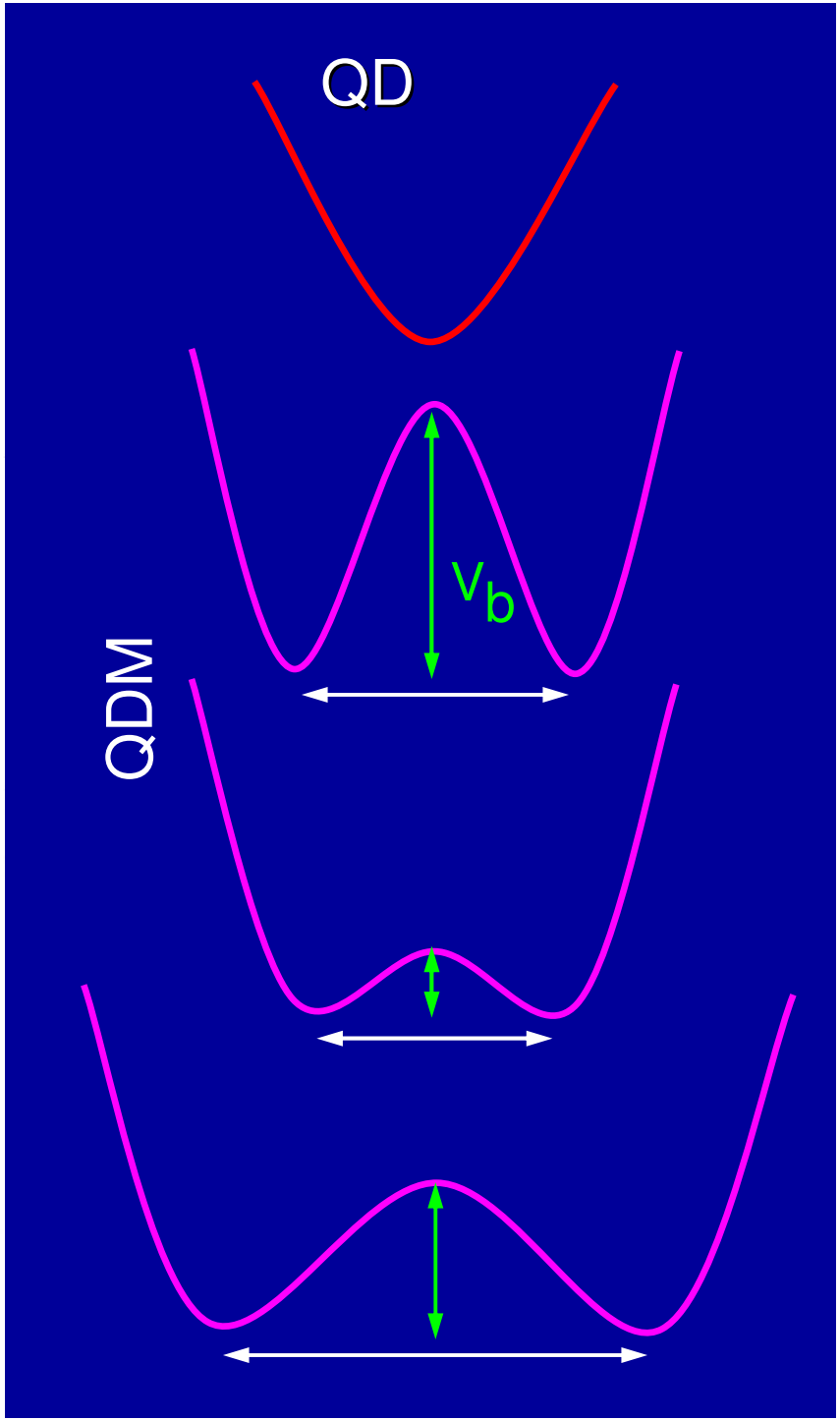
$$[(\vec{p}_i - e\vec{A}_i/c)^2 - \vec{p}_i^{\,2}]/2m^* + g^* \mu_B \vec{B}\cdot\vec{S}_i/\hbar$$

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

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

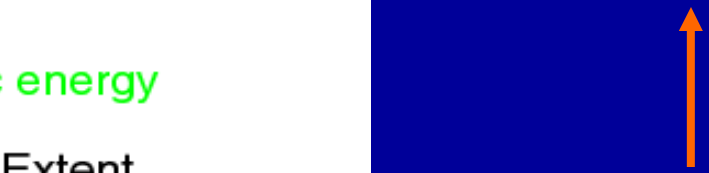
$\hbar\omega_0$ (5 - 1 meV) => R_W (1.48 - 3.31)

- 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)

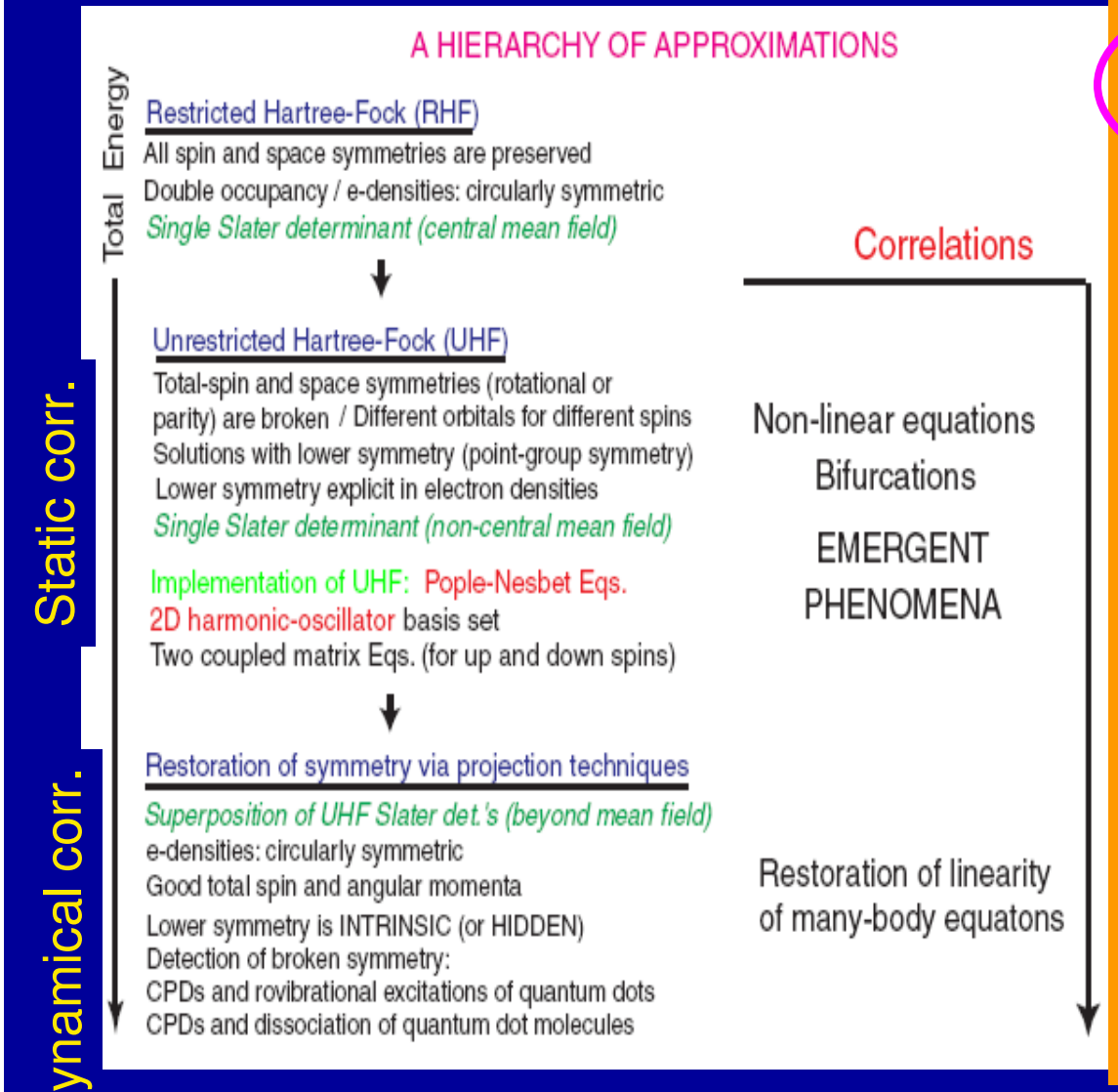
$$R_\delta = gm/(2\pi\hbar^2)$$



Neutral bosons

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)

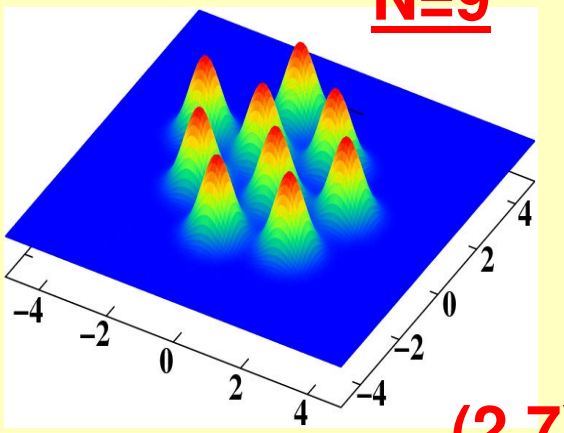
$$|\Phi_N^{\mathrm{UBHF}}\rangle \propto$$

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

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

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

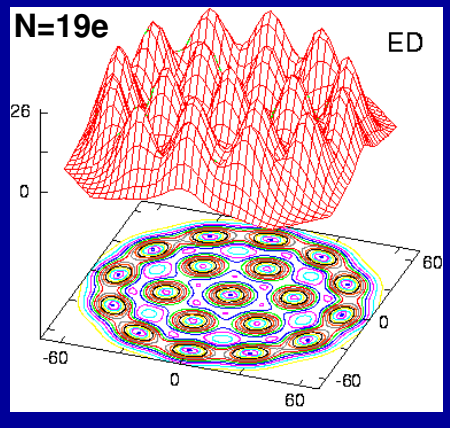
N=9



(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).



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

Restoration of Broken Rotational Symmetry

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

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

- 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.

$R_\delta = 50$

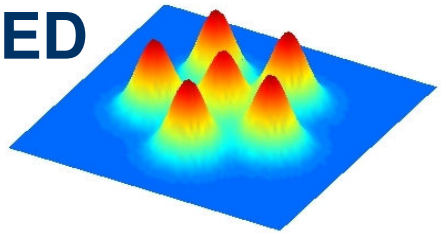
Rotating Frame

$R_W = 10$

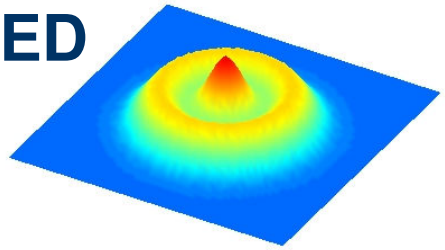
Magnetic Field

Probability densities

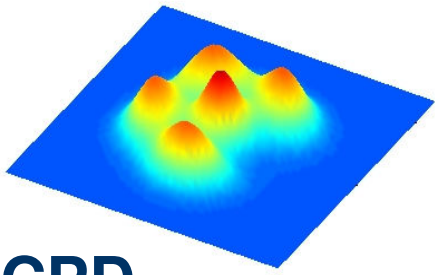
ED

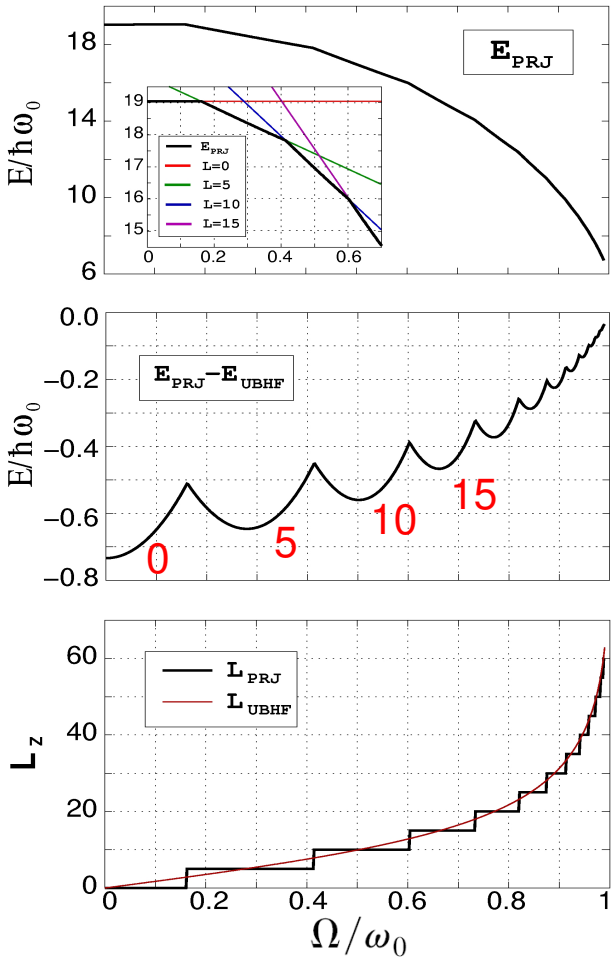


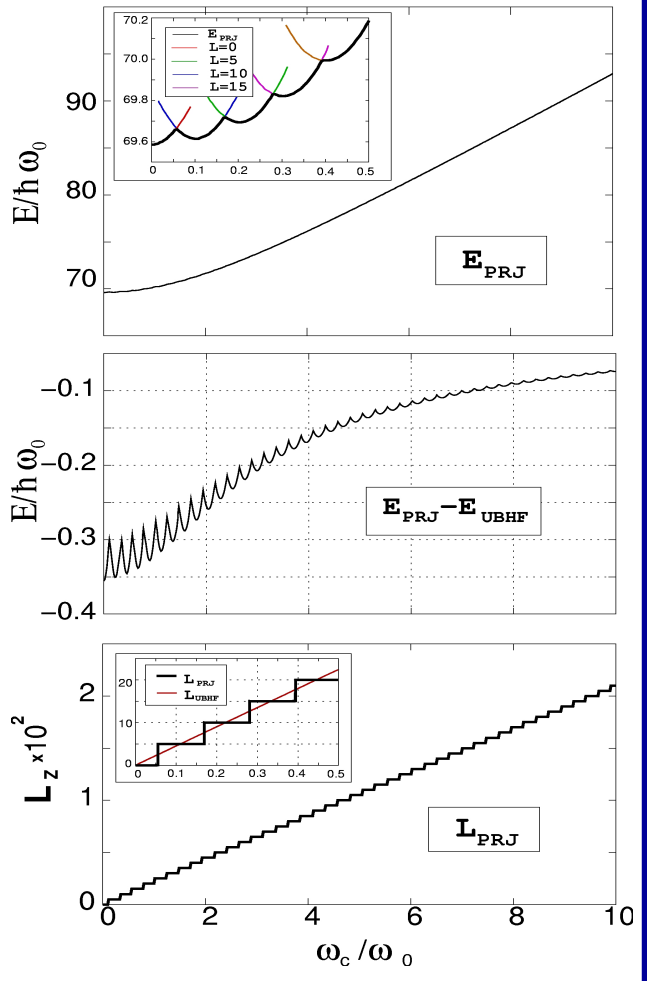
ED



CPD







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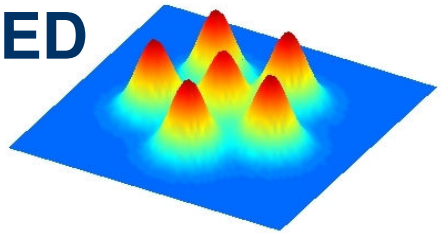
Rotating Frame

R_W =10

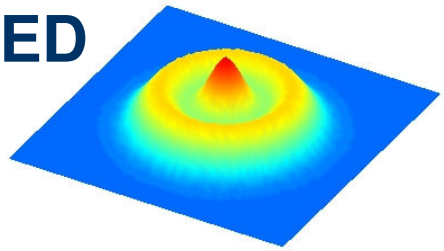
Magnetic Field

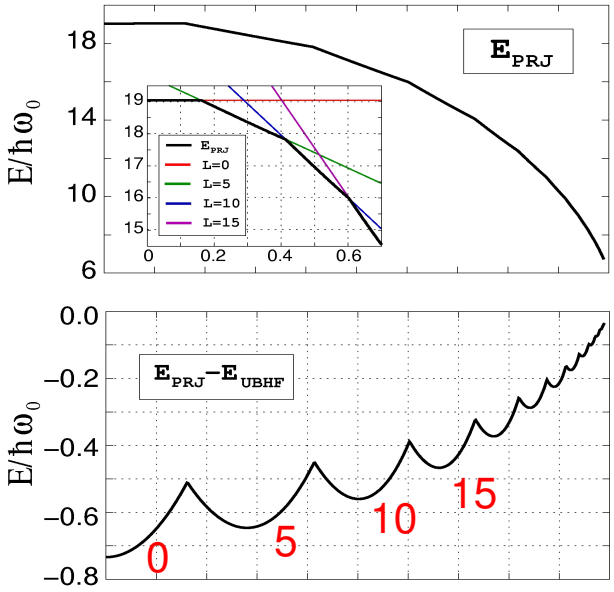
Probability densities

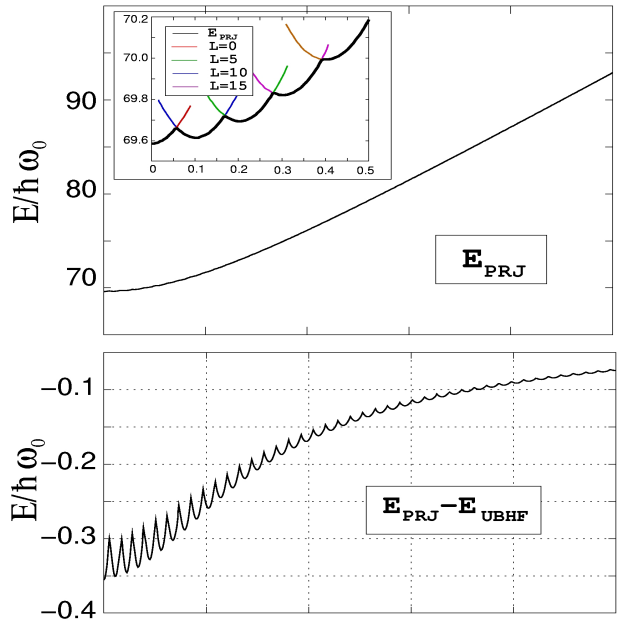
ED



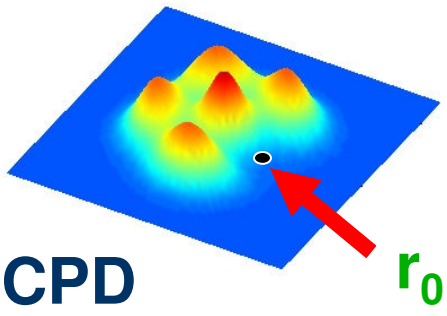
ED







CPD



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

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

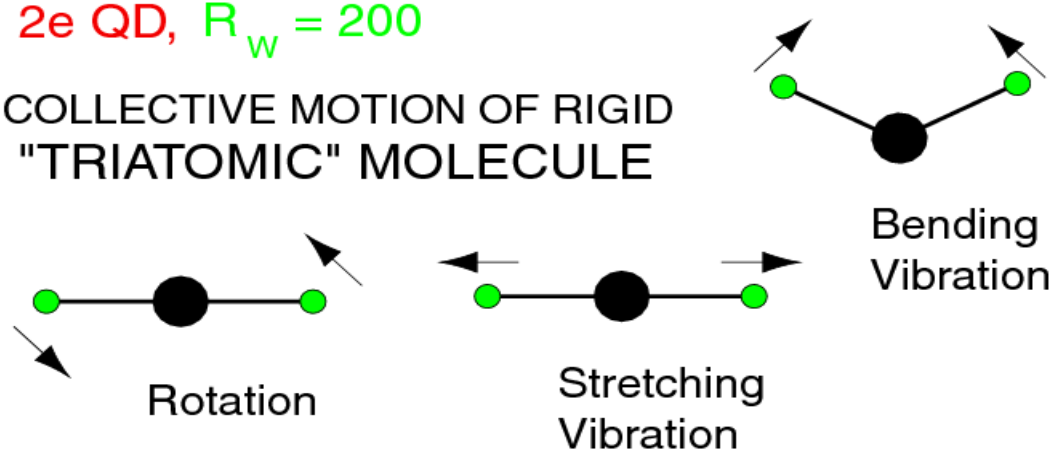
Exact

Y&L, PRL 85, 1726 (2000)

Quantum Dot Helium

2e QD, $R_w = 200$

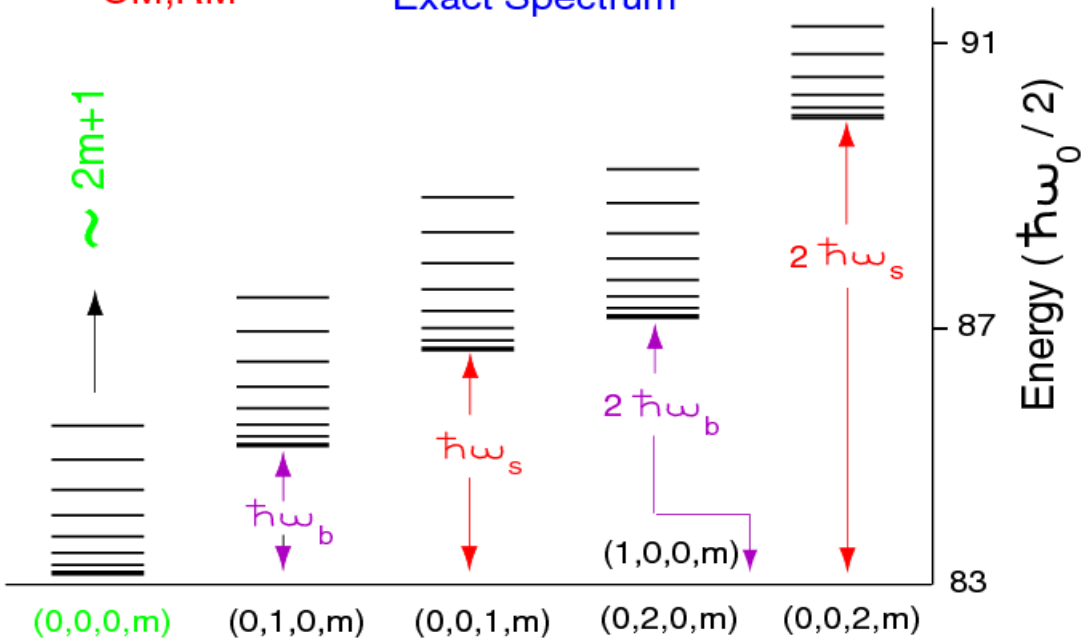
COLLECTIVE MOTION OF RIGID "TRIATOMIC" MOLECULE



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

CM,RM

Exact Spectrum



RIGID ROTOR

B=0

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

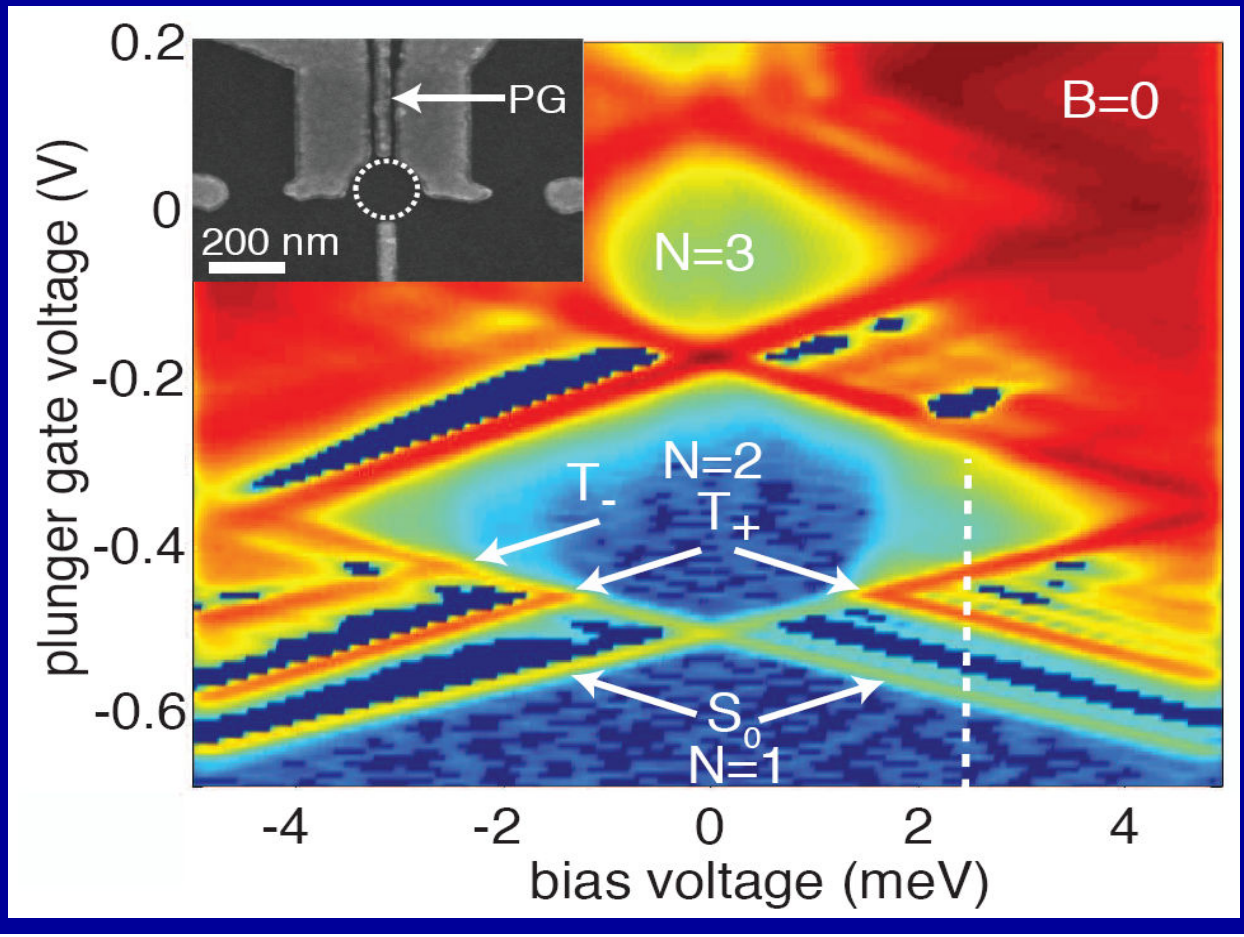
C. Ellenberger et al., Phys. Rev. Lett. **96,** 126806 (2006)

(No Zeeman splitting)

N=2e

η= 0.72

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



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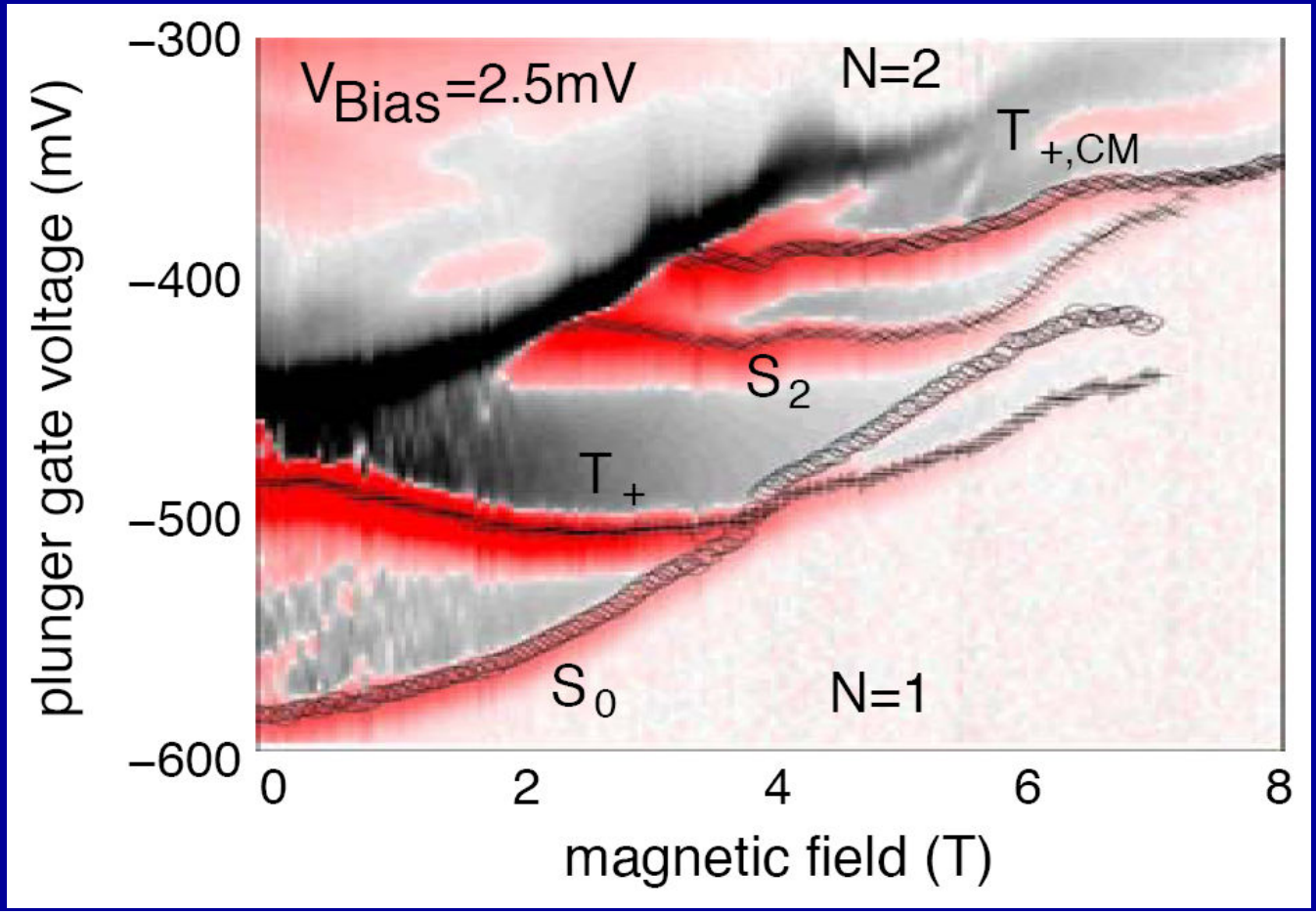
C. Ellenberger et al., Phys. Rev. Lett. **96,** 126806 (2006)

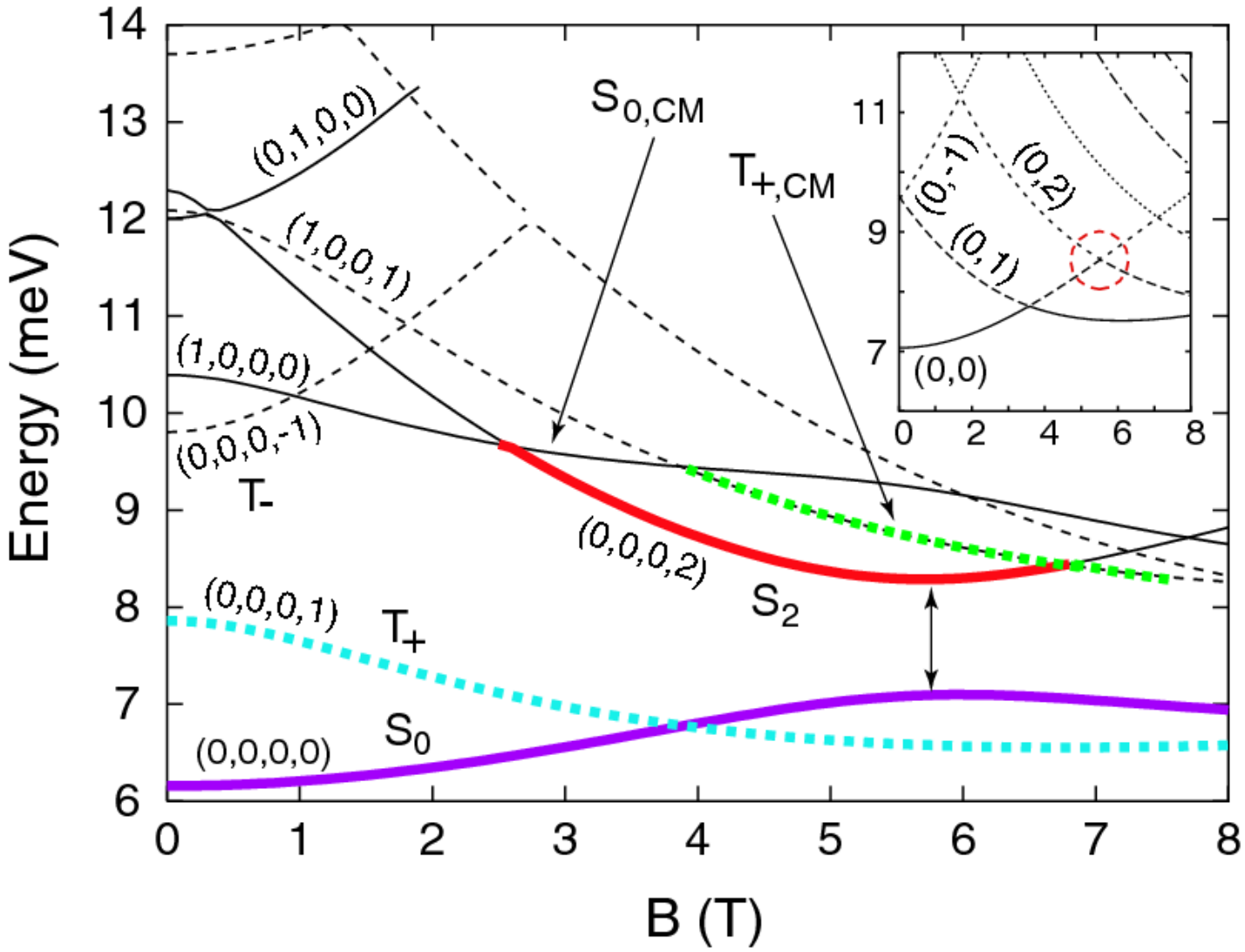
(No Zeeman splitting)

ETH Zurich single QD



ETH single QD

EXD = Exact diagonalization



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:

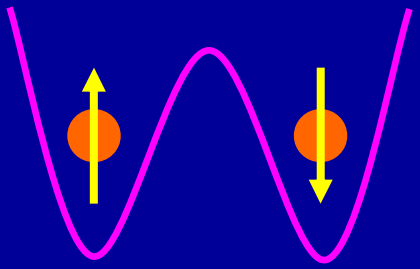
$$\Psi^s_{\mathrm{GVB}}(1,2) = n_s \sqrt{2} P_0 \Psi_{\mathrm{UHF}}(1,2)$$ ← singlet

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

GVB, Generalized Valence Bond
GHL, Generalized Heitler London

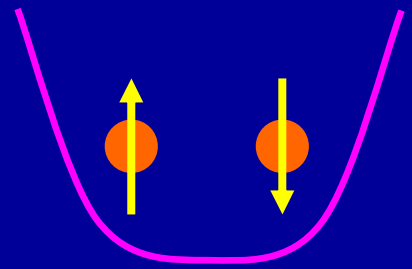
Y&L, Eur. Phys. J. D 16, 373 (2001)
Int. J. Quantum Chem. 90, 699 (2002)

DQD



localized orbitals

Elongated QD



No circular symmetry

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

4.23 meV

5.84 meV

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

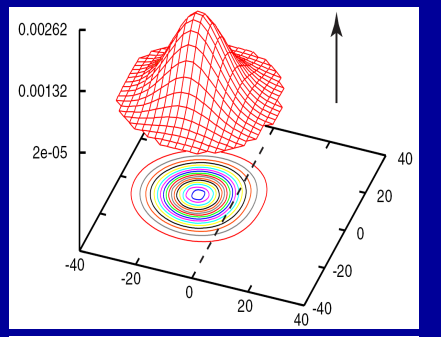
N=2e

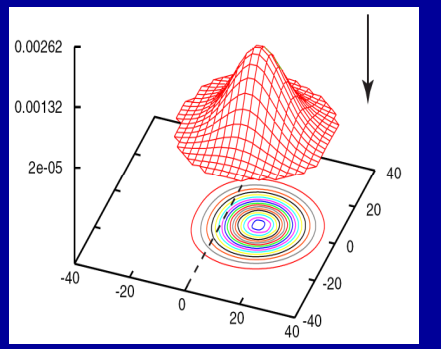
$$T = (\mathbf{p} - e\mathbf{A}/c)^2/2m^*, \text{ with } \mathbf{A} = 0.5(-By, Bx, 0)$$

B=3.8 T

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

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



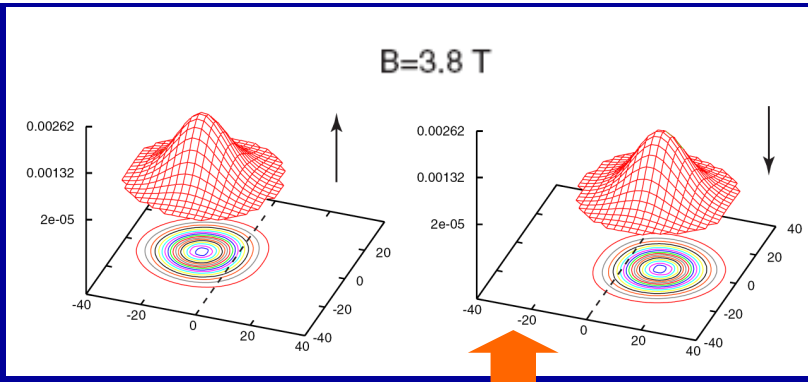


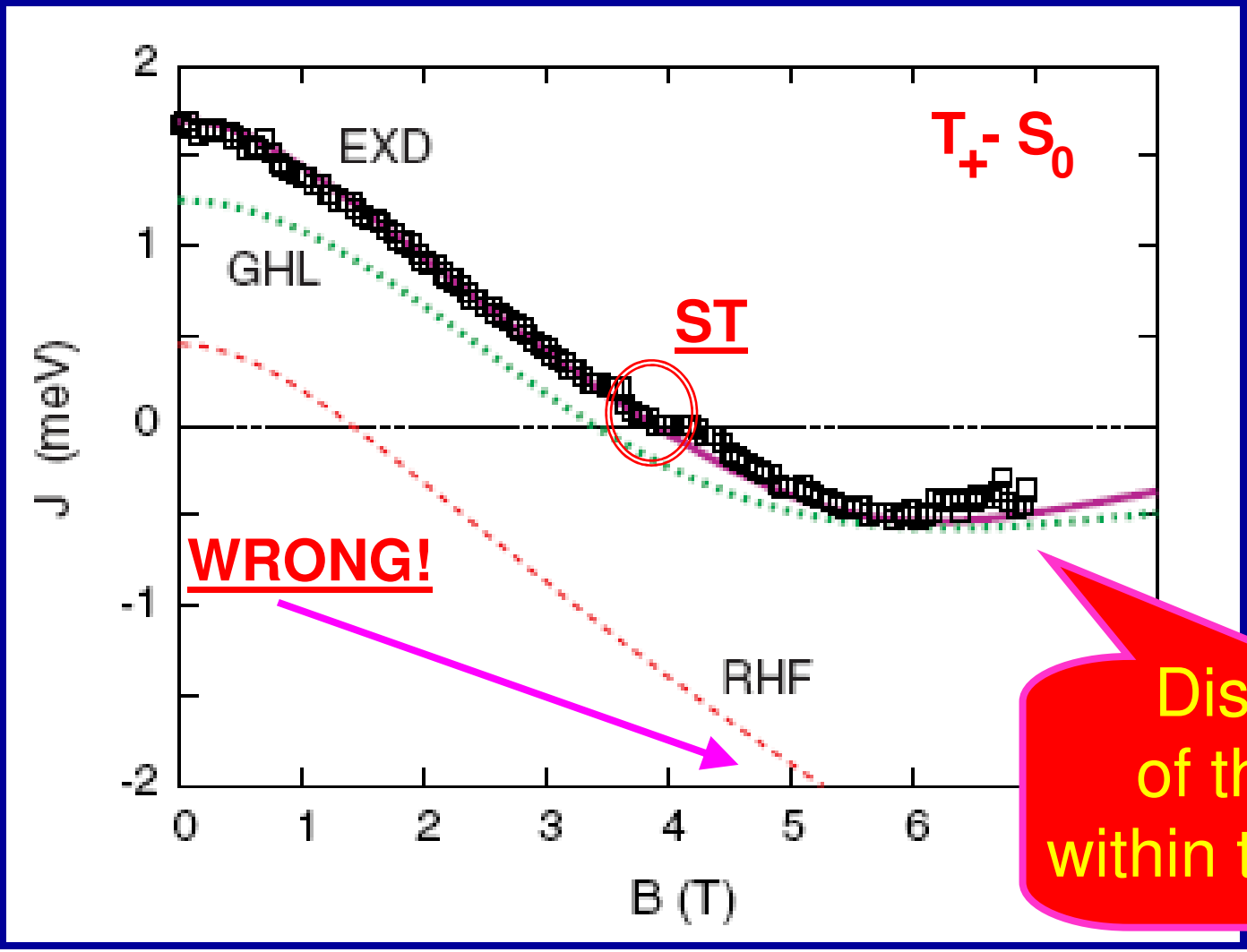
$$\Psi^{s,t}_{\mathrm{GHL}}(\mathbf{r}_1, \mathbf{r}_2) \propto \left(u_L(\mathbf{r}_1)u_R(\mathbf{r}_2) \pm u_L(\mathbf{r}_2)u_R(\mathbf{r}_1)\right)\chi^{s,t}$$

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





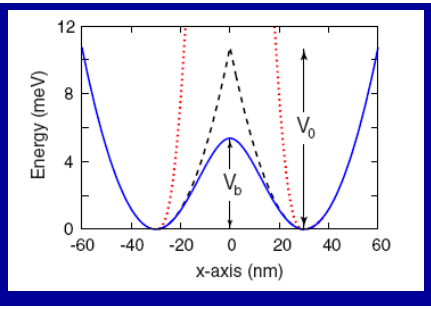
UHF broken symmetry orbitals used to construct the GHL wave function

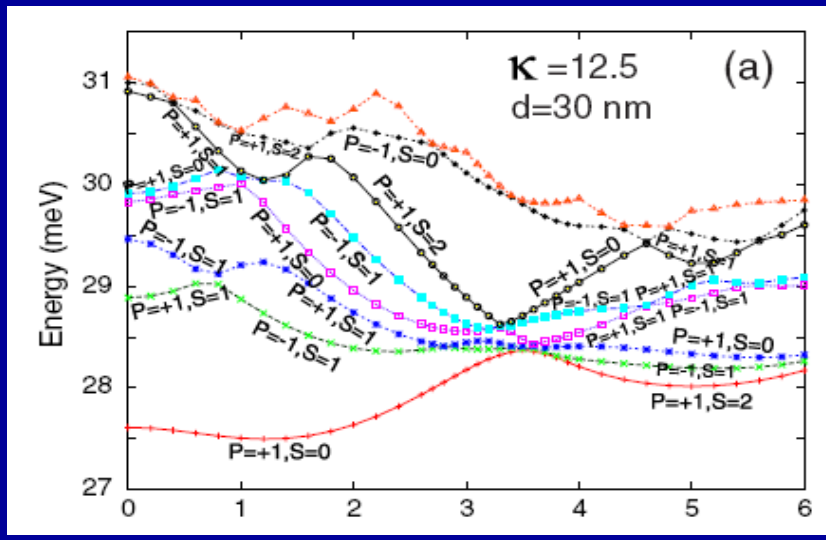
Dissociation of the 2e WM within the single QD

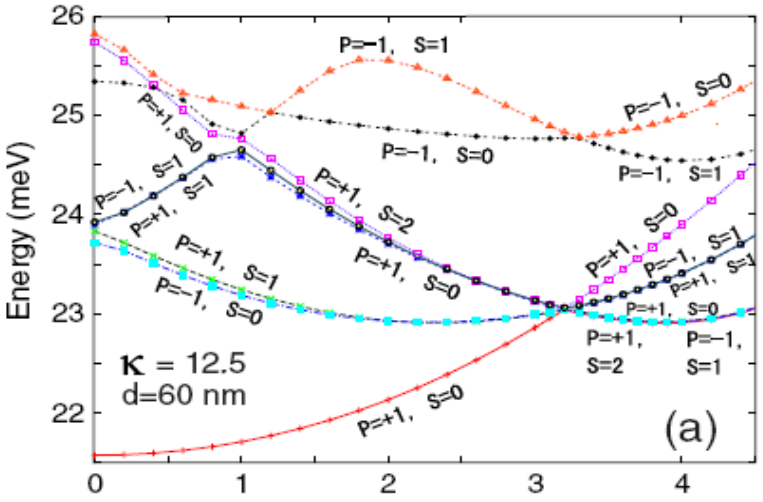
Quantum Dot Helium Molecule

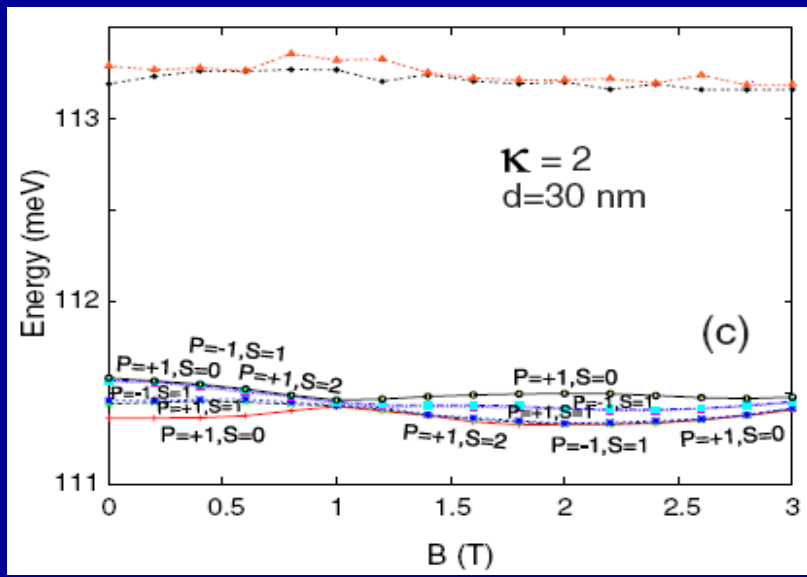
Ying Li, Y&L, Phys. Rev. B 80, 045326 (2009)

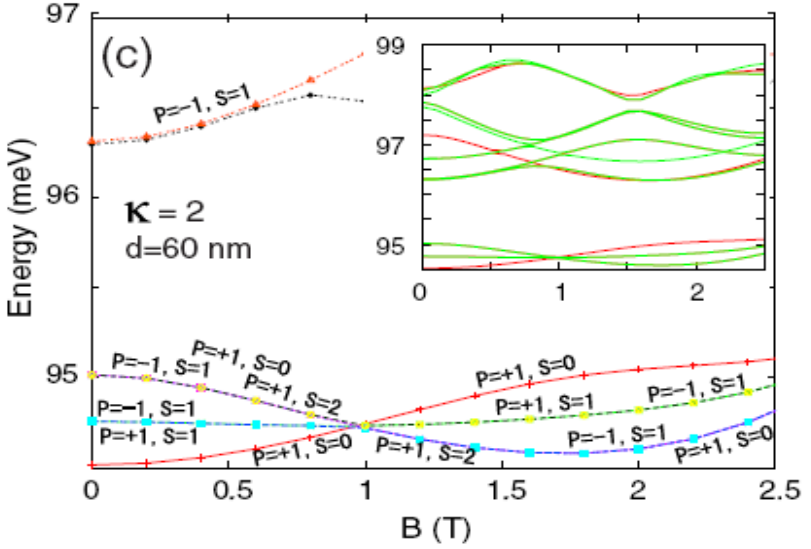
EXD calculation







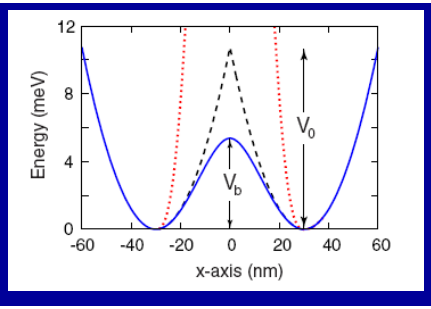


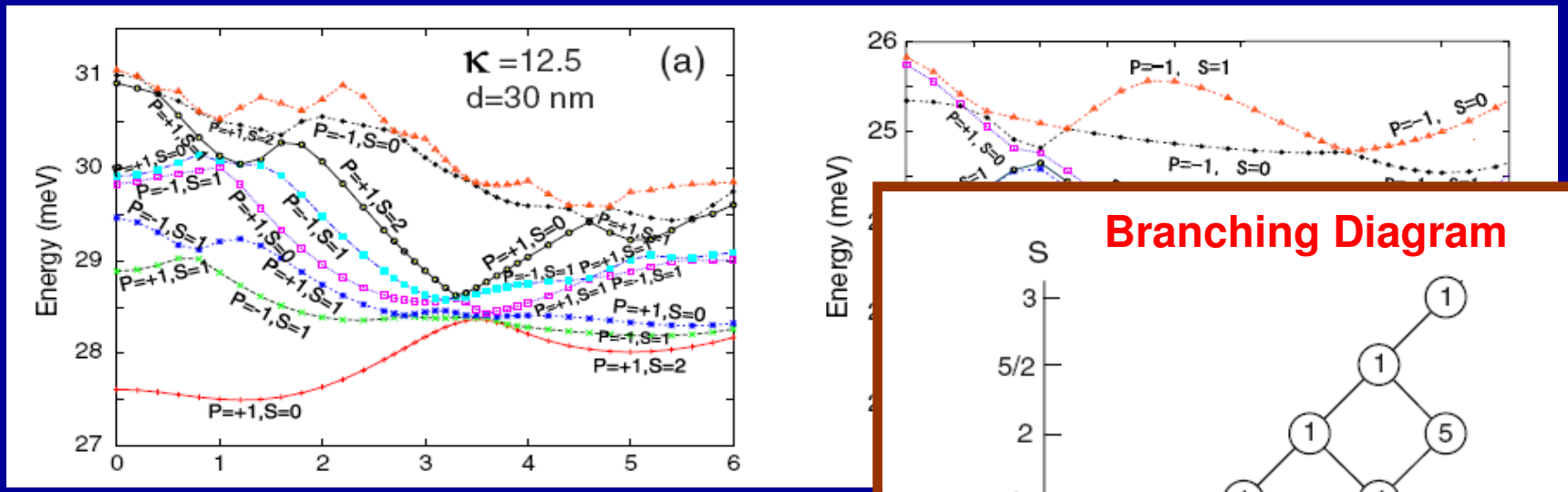


Quantum Dot Helium Molecule

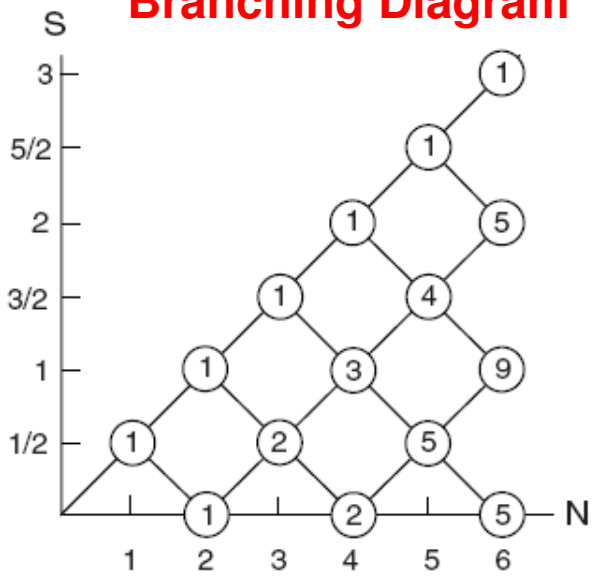
Ying Li, Y&L, Phys. Rev. B 80, 045326 (2009)

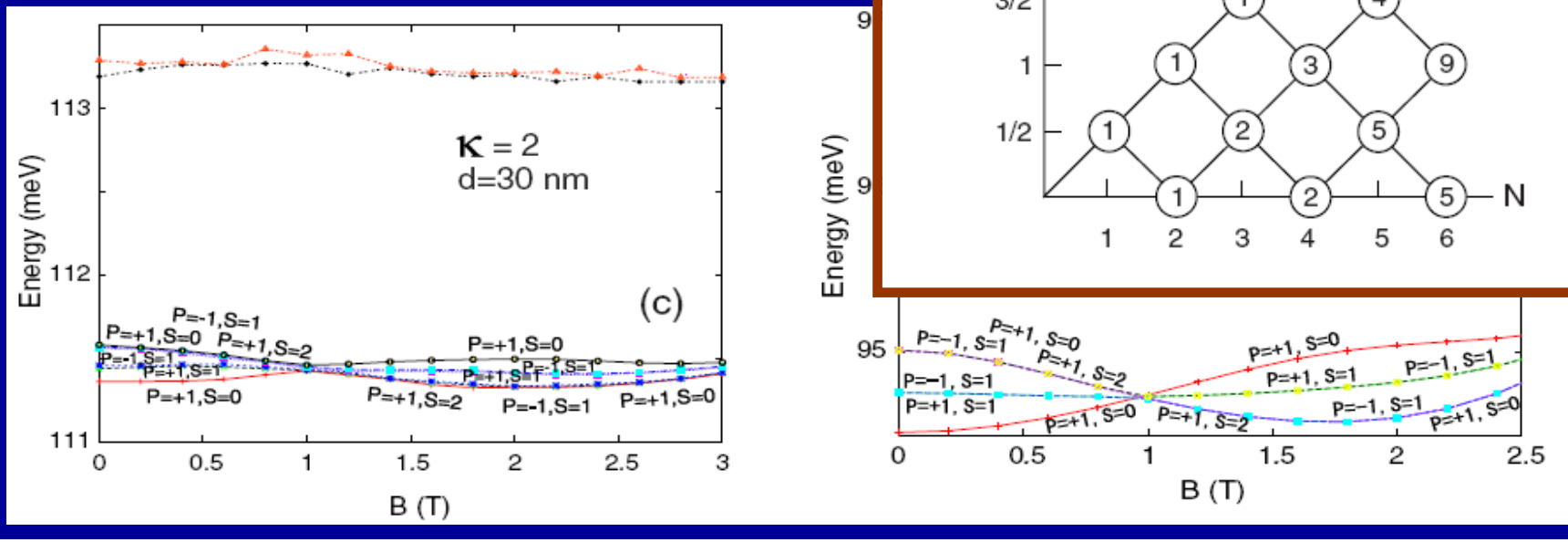
EXD calculation





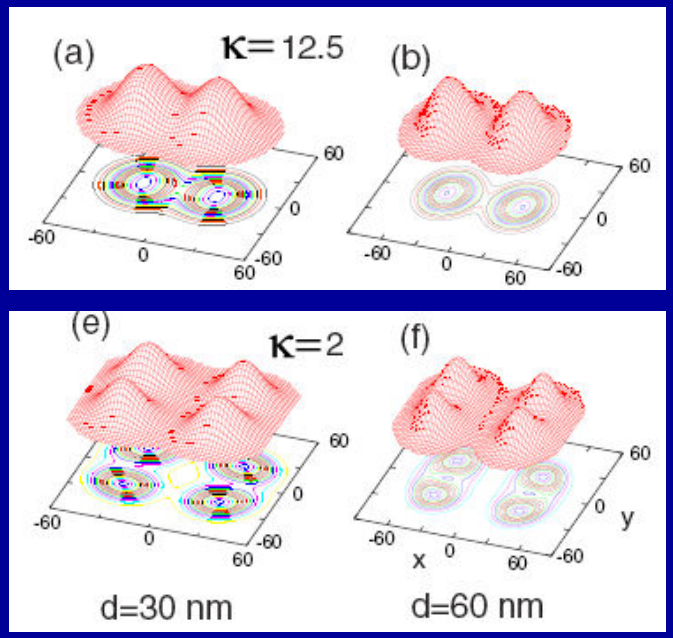
Branching Diagram



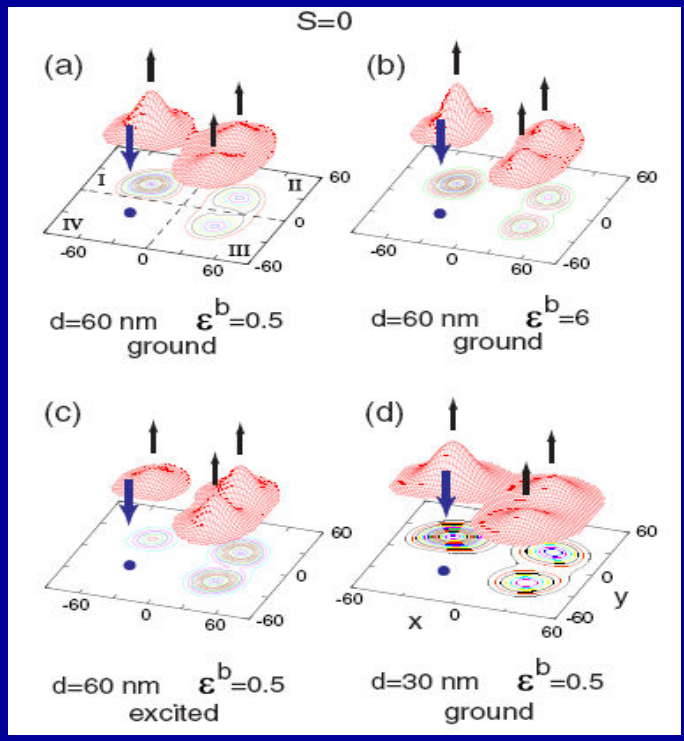


States at B=0 $S = 0, S_z = 0$

Ground State Electron Densities



Spin-resolved Pair Correlations



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

I ~ 100,000

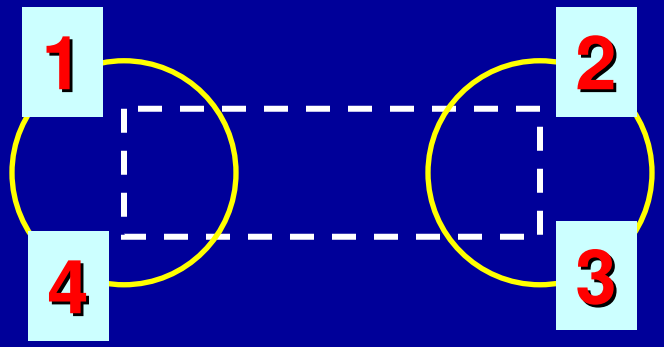
Slater Determinant

Spin functions

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

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

4-site Heisenberg cluster



No itinerant ferromagnetism

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

$$S_z = 0$$

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

$|1\rangle \rightarrow |\uparrow\uparrow\downarrow\downarrow\rangle$ $|2\rangle \rightarrow |\uparrow\downarrow\uparrow\downarrow\rangle$ ..... $|6\rangle \rightarrow |\downarrow\downarrow\uparrow\uparrow\rangle$

A universal molecular description for the spectra of bosons and fermions in the lowest Landau level (SOFT ROTOR)

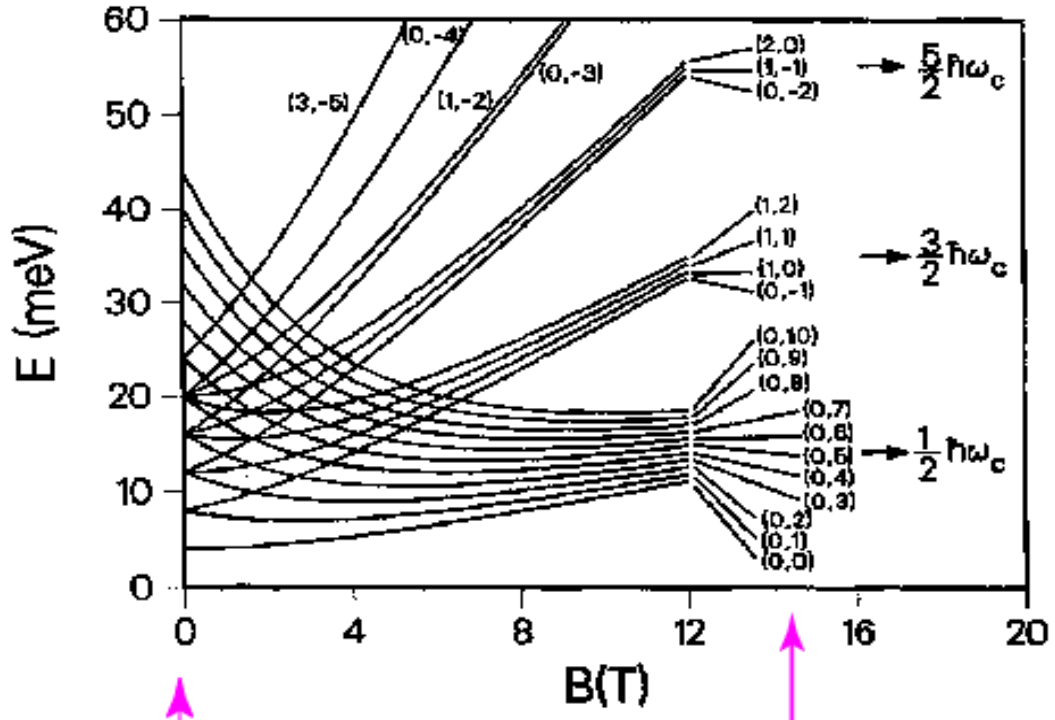
Constantine Yannouleas and Uzi Landman,
Phys. Rev. A 81, 023609 (2010)

Reminder: Zero magnetic field or no rotation leads to a **rigid rotor** for strong interparticle repulsion

Circular 2D QD NO e-e INTERACTION

DARWIN-FOCK S.P. LEVELS AT ANY B

NO MAGNETIC FIELD



STRONG MAGNETIC FIELD

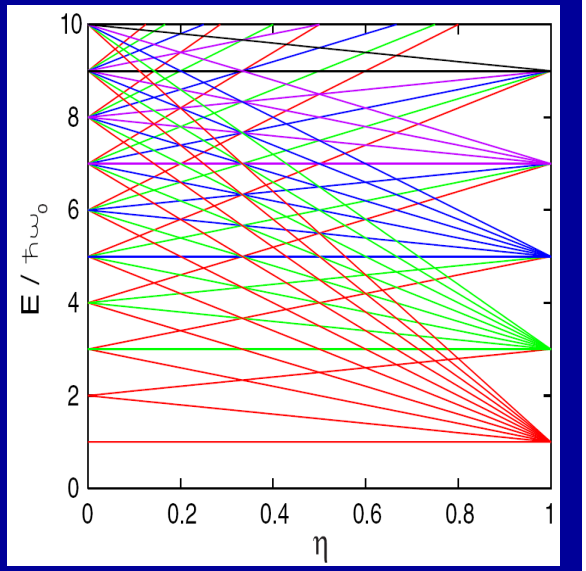
Closed Shells:
2, 6, 12, 20, ...

Landau levels
Full polarization
Open shells

Fractional Quantum Hall Effect

B -> Omega

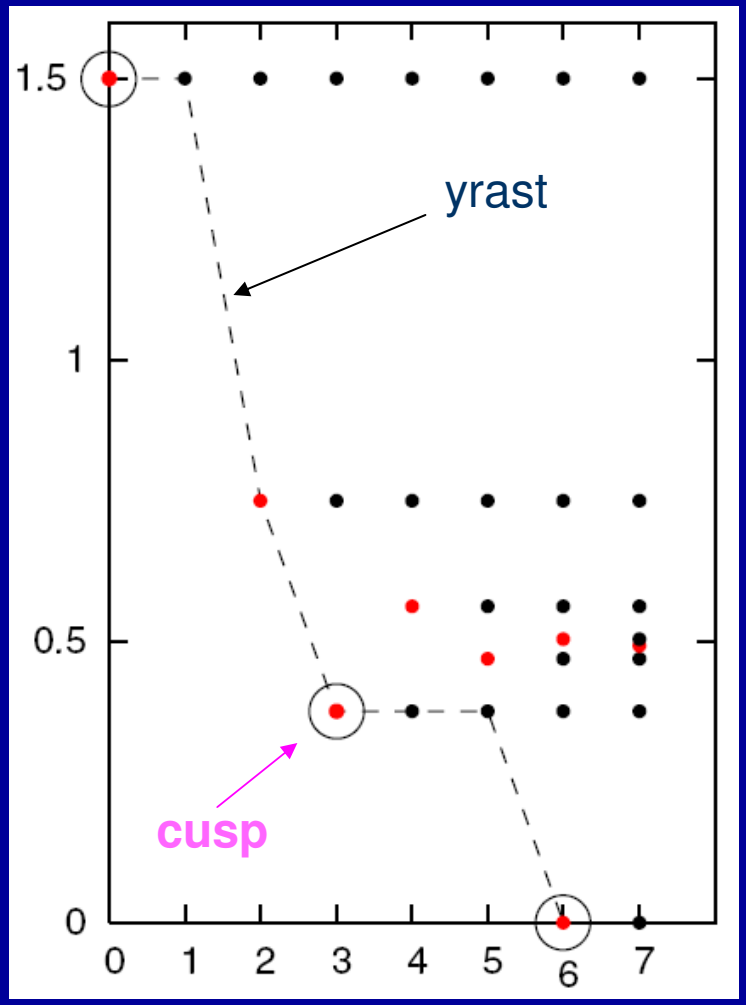
Rotating atomic traps



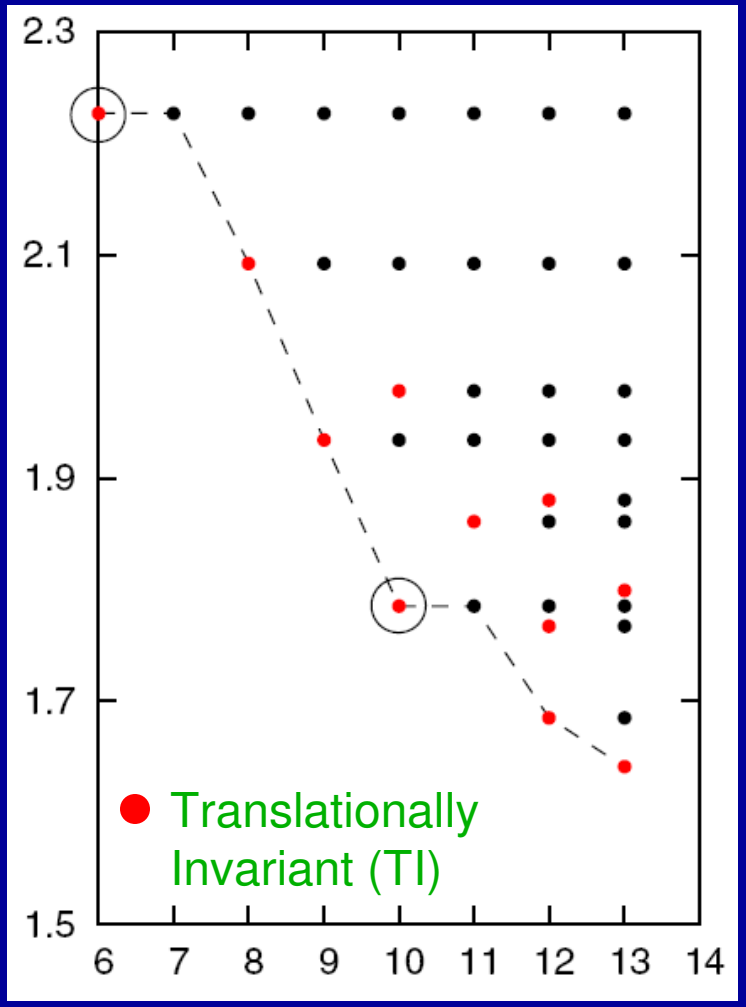
$$\eta = \Omega/\omega_0$$

Full LLL spectra (interaction only)

N=3 bosons (delta)



N=4 fermions (Coulomb)



Energy

L

L

RVM trial functions:

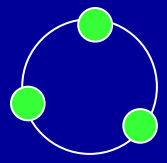
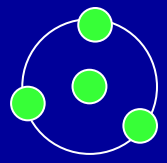
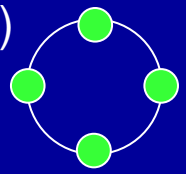
RXM -> RBM or REM

$$\Phi_{\mathcal{L}}^{\mathrm{RXM}}(n_1,n_2)Q_\lambda^m|0>$$

$$L=\mathcal{L}+\lambda m$$

Pure rotations (cusp, vibrationless)

(molecular point-group symmetries)

(0,3)  (1,3)  (0,4) 

RBM

$$\Phi_{\mathcal{L}}^{\mathrm{RBM}}(0,3)=\sum_{0\le l_1\le l_2\le l_3}^{l_1+l_2+l_3=\mathcal{L}} C(l_1,l_2,l_3)\ \mathrm{Perm}[z_1^{l_1},z_2^{l_2},z_3^{l_3}]$$

$$C(l_1,l_2,l_3) = \left(\prod_{i=1}^{3} l_i!\right)^{-1}\left(\prod_{k=1}^{M} p_k!\right)^{-1} \times\left(\sum_{1\le i<j\le 3}\cos\left[\frac{2\pi(l_i-l_j)}{3}\right]\right)$$

$$\mathcal{L}=\mathcal{L}_0+n_1k_1+n_2k_2$$

MAGIC ANGULAR MOMENTA

Vibrations

$$Q_\lambda=\sum_{i=1}^{N}(z_i-z_c)^\lambda$$

$$z_c=(1/N)\sum_{i=1}^{N} z_i$$

REMs (analytic):
Yannouleas and Landman,
PRB 66, 115315 (2002);
Rep. Prog. Phys. 70, 2067 (2007)

SUMMARY (Symmetry Restoration)

Under appropriate conditions, 2D electrons (and ultracold repelling bosons) do localize and organize themselves in geometric shells, forming
Rotating (or pinned) Wigner Molecules
(semiconductor and graphene Quantum Dots,
Ultracold rotating bosonic traps)

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