Few-electron anisotropic QDs in low magnetic fields: exact-diagonalization results for excitations, spin configurations, and entanglement

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N=2e: C. Ellenberger et al, PRL **96**, 126806 (2006)

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

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

WAVE-FUNCTION BASED APPROACHES

TWO-STEP METHOD

A HIERARCHY OF APPROXIMATIONS

Total Energy

Static corr.

Restricted Hartree-Fock (RHF)

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

↓

Unrestricted Hartree-Fock (UHF)

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

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

↓

Dynamical corr.

Restoration of symmetry via projection techniques

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

Correlations

Non-linear equations
Bifurcations

EMERGENT PHENOMENA

Restoration of linearity of many-body equatons

EXACT DIAGONALIZATION

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)*

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

1) *Detailed description of excitation spectra (advantage over DFT, etc…)* [first part]

2) *Description of many-body entanglement (advantage over DFT, etc…)* [first part]

3) *Transport properties in QDs (current intensity, phase lapses in Aharonov-Bohm interferometry)* [second part]

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

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

EXD:

$$\mathcal{H} = \sum_{i=1}^{N} [\mathbf{p}_i^2/(2m^*) + V(x_i, y_i)] + \sum_{i<j} e^2/(\kappa r_{ij})$$

$$V(x,y) = m^*(\omega_x^2 x^2 + \omega_y^2 y^2)/2$$

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

I ~ 100,000

Slater determinant

How does one describe entanglement in EXD wfs?

(a) Measure of entanglement: Von Neumann entropy

$$\mathcal{S}_{\mathrm{vN}} = -\mathrm{Tr}(\rho \log_2 \rho) + \mathcal{C},$$

$$\mathcal{C} = -\log_2 N$$

Measure of how many determinants

$$\rho_{\nu\mu} = \frac{\langle \Psi^{\mathrm{EXD}} | a_\mu^\dagger a_\nu | \Psi^{\mathrm{EXD}} \rangle}{\sum_\mu \langle \Psi^{\mathrm{EXD}} | a_\mu^\dagger a_\mu | \Psi^{\mathrm{EXD}} \rangle}$$

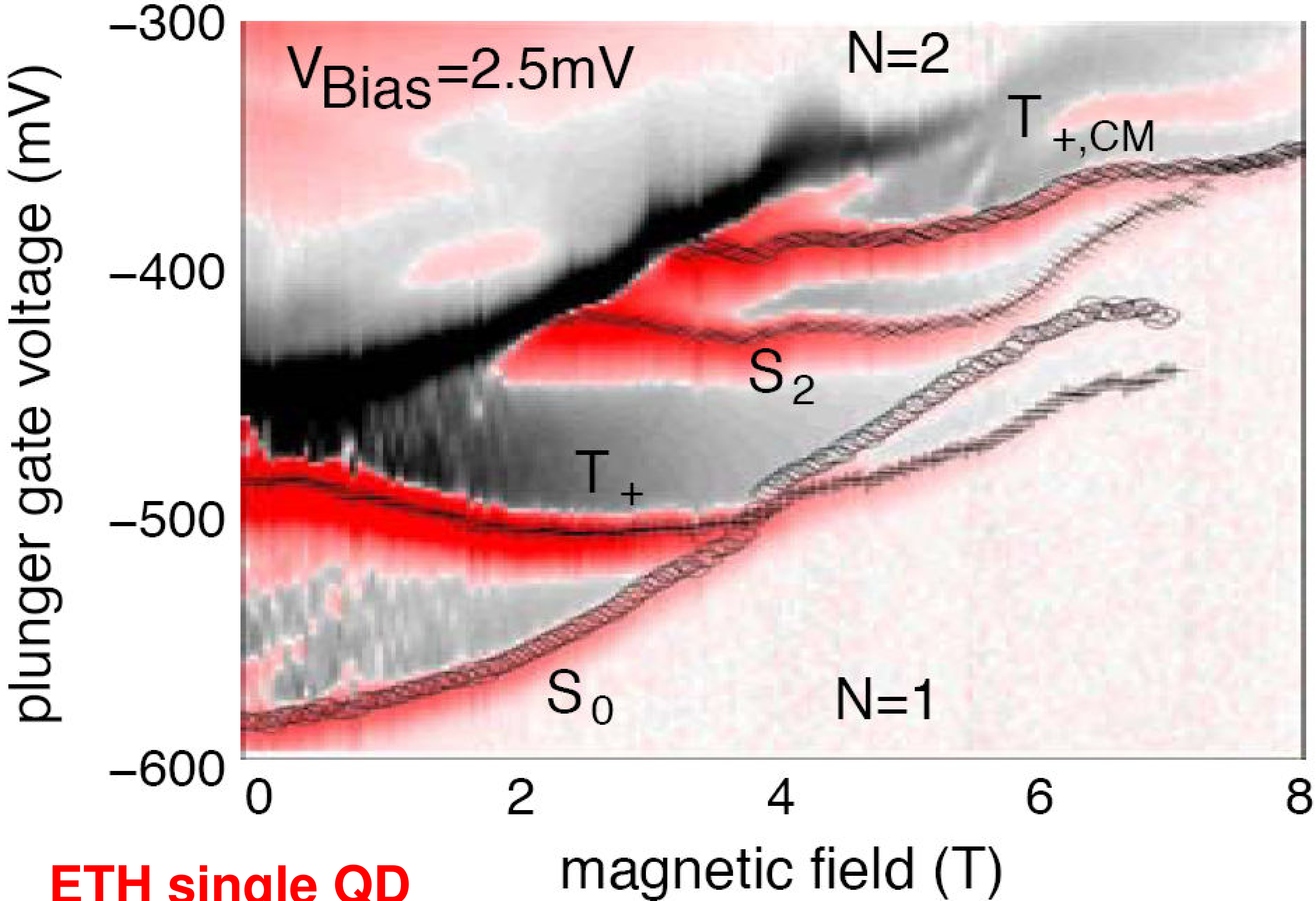
$$\langle \Psi^{\mathrm{EXD}} | a_\mu^\dagger a_\nu | \Psi^{\mathrm{EXD}} \rangle = \sum_{I,J} C_I^* C_J \langle \mathrm{SD}(I) | a_\mu^\dagger a_\nu | \mathrm{SD}(J) \rangle$$

Excitation spectrum of two correlated electrons in a lateral quantum dot with negligible Zeeman splitting

C. Ellenberger, T. Ihn (ETH, Zurich),
K. Ensslin (ETH, Zurich),
C. Yannouleas, Uzi Landman,
D. Driscoll, A.C. Gossard (Santa Barbara)

Phys. Rev. Lett. ***96,*** *126806 (2006)*

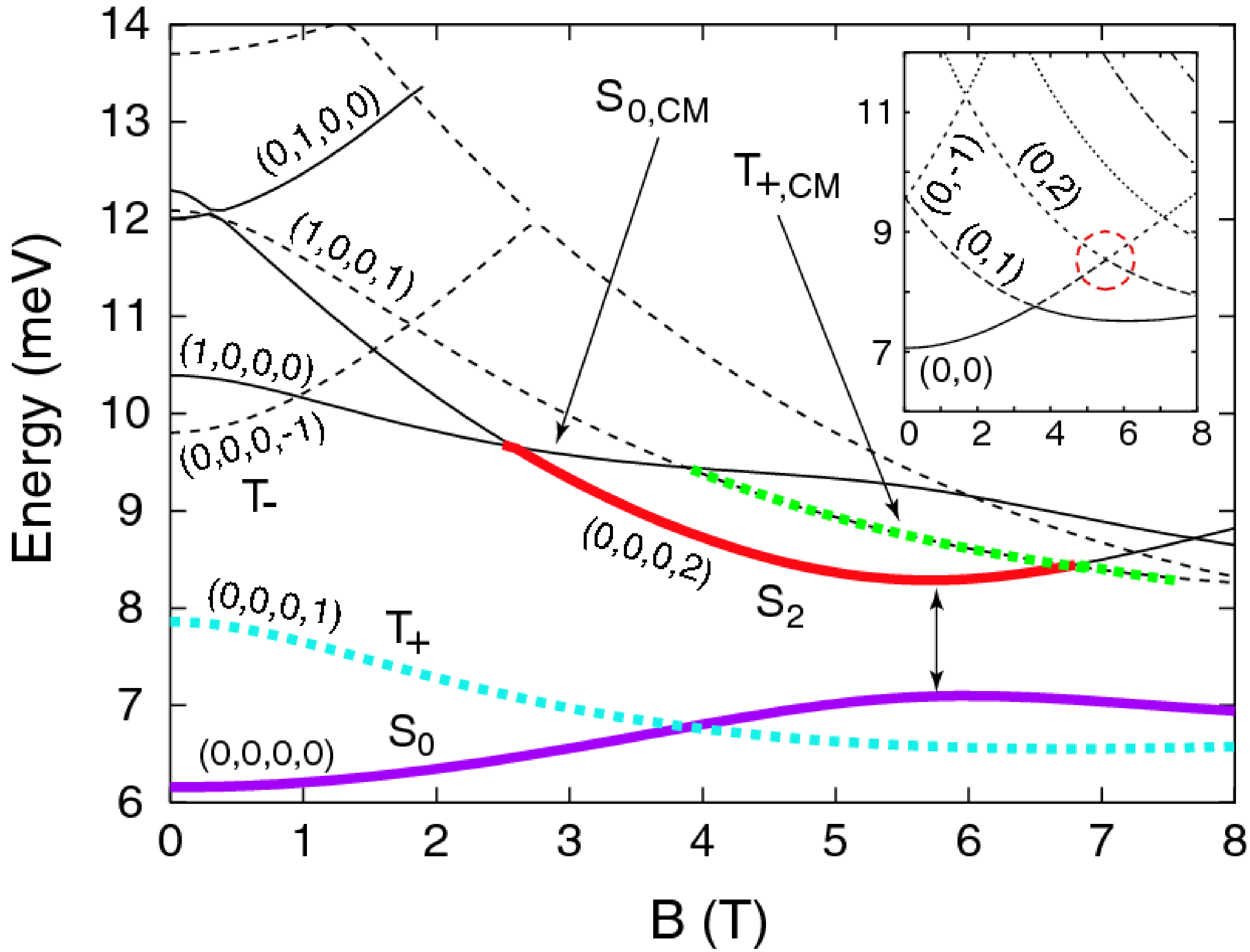
(Anisotropic Quantum Dot Helium)



ETH single QD

ETH single QD

EXD = Exact diagonalization



"THE WAY DOWN" TWO-STEP METHOD

SECOND STEP:
RESTORATION OF SYMMETRIES VIA PROJECTION

TOTAL SPIN:

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

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

↑ interchanges spins

Two electrons in a DQD:

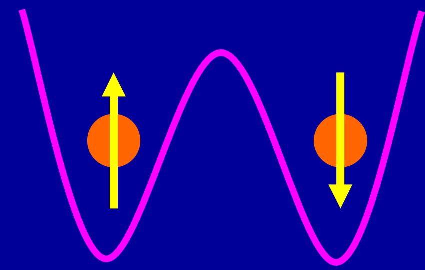
$$\Psi^{s}_{\mathrm{GVB}}(1,2) = n_s \sqrt{2} P_0 \Psi_{\mathrm{UHF}}(1,2)$$ ← singlet

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

GVB, Generalized Valence Bond
GHL, Generalized Heitler London

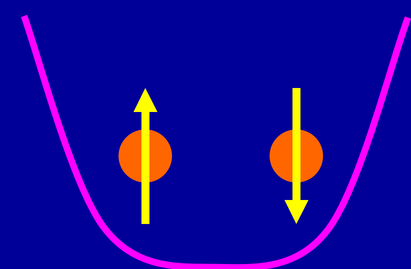
Y&L, Eur. Phys. J. D 16, 373 (2001)
Int. J. Quantum Chem. 90, 699 (2002)

DQD



localized orbitals

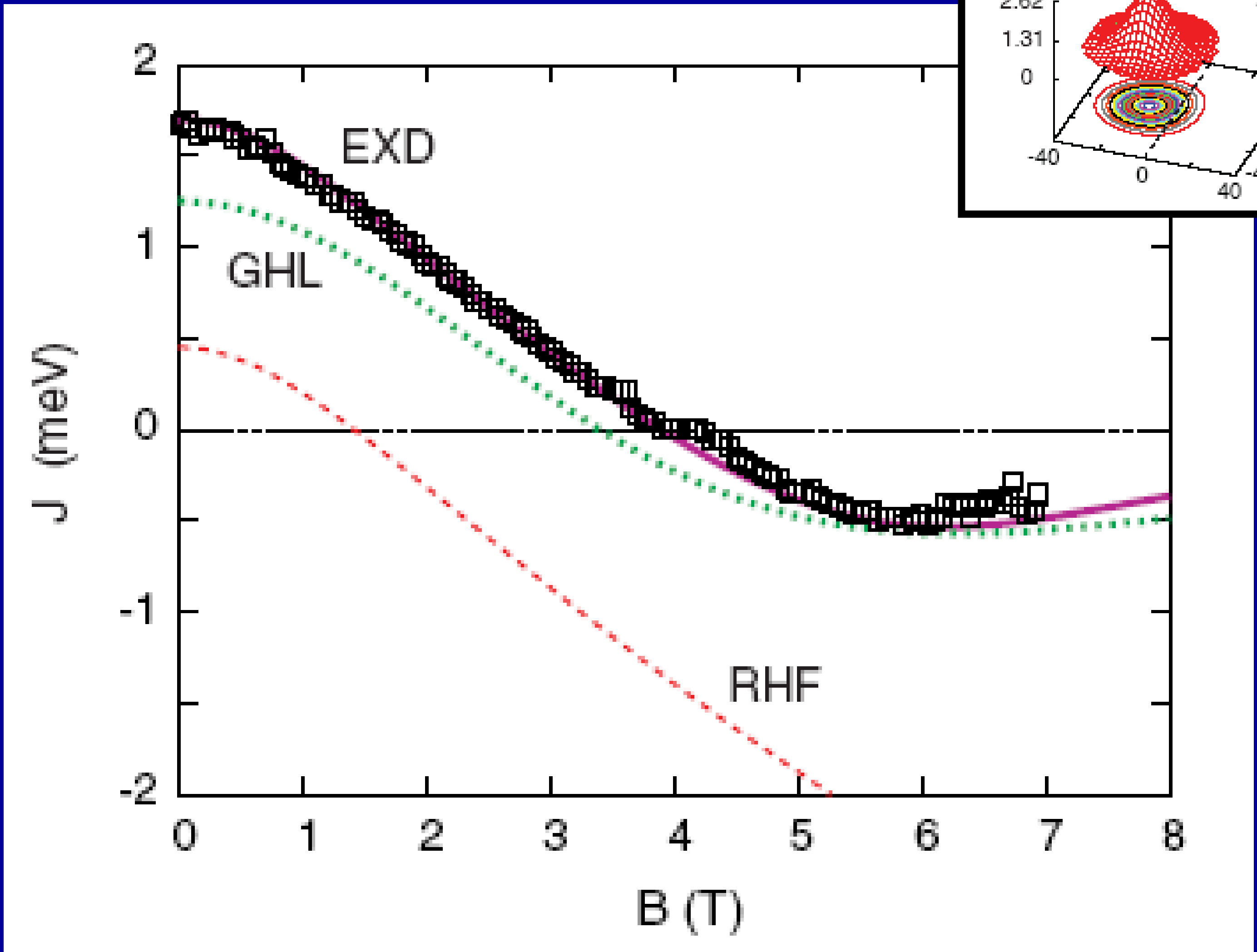
Elongated QD

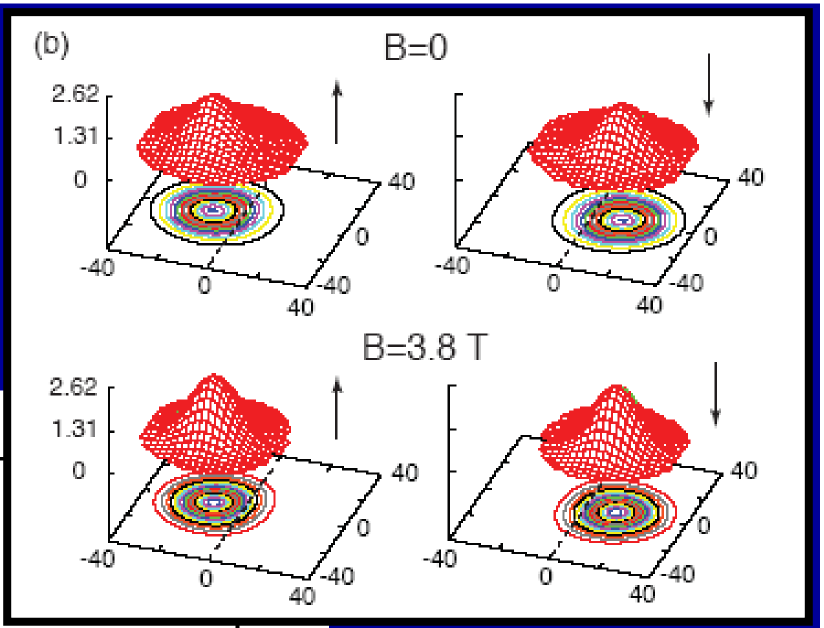


1) Symmetry breaking
2) Symmetry restoration

ETH single QD

hwx=4.23 meV; hwy=5.84 meV;
m*=0.070; kappa=12.5; a=0.86





UHF broken symmetry orbitals used to construct the GHL wave function

2e elliptic QD

Exact

$$\Psi^{s,t}_{\rm EXD}(\mathbf{r}_1,\mathbf{r}_2) = \sum_{i<j}^{2K} \Omega^{s,t}_{ij} |\psi(1;i)\psi(2;j)\rangle$$

Canonical form:

Exact

$$\Psi^{s,t}_{\rm EXD}(\mathbf{r}_1,\mathbf{r}_2) = \sum_{k=1}^{M} z^{s,t}_k |\Phi(1;2k-1)\Phi(2;2k)\rangle.$$

K=79; M <= K

GHL $$\Psi^{s}_{\rm GHL} \propto |\Phi^+(1\uparrow)\Phi^+(2\downarrow)\rangle - \eta|\Phi^-(1\uparrow)\Phi^-(2\downarrow)\rangle.$$ Singlet

GHL $$\Psi^{t}_{\rm GHL} \propto |\Phi^+(1\uparrow)\Phi^-(2\downarrow)\rangle + |\Phi^+(1\downarrow)\Phi^-(2\uparrow)\rangle$$ Triplet

ETH single QD

Measure of Entanglement

(Quantum Computing)

Von Neumann Entropy
(indistinguishable parties)

$$S = -\sum_{k=1}^{M} |z_k|^2 \log_2(|z_k|^2)$$

$$\Psi^{s,t}_{\rm EXD}({\bf r}_1,{\bf r}_2) = \sum_{i<j}^{2K} \Omega^{s,t}_{ij} |\psi(1;i)\psi(2;j)\rangle$$

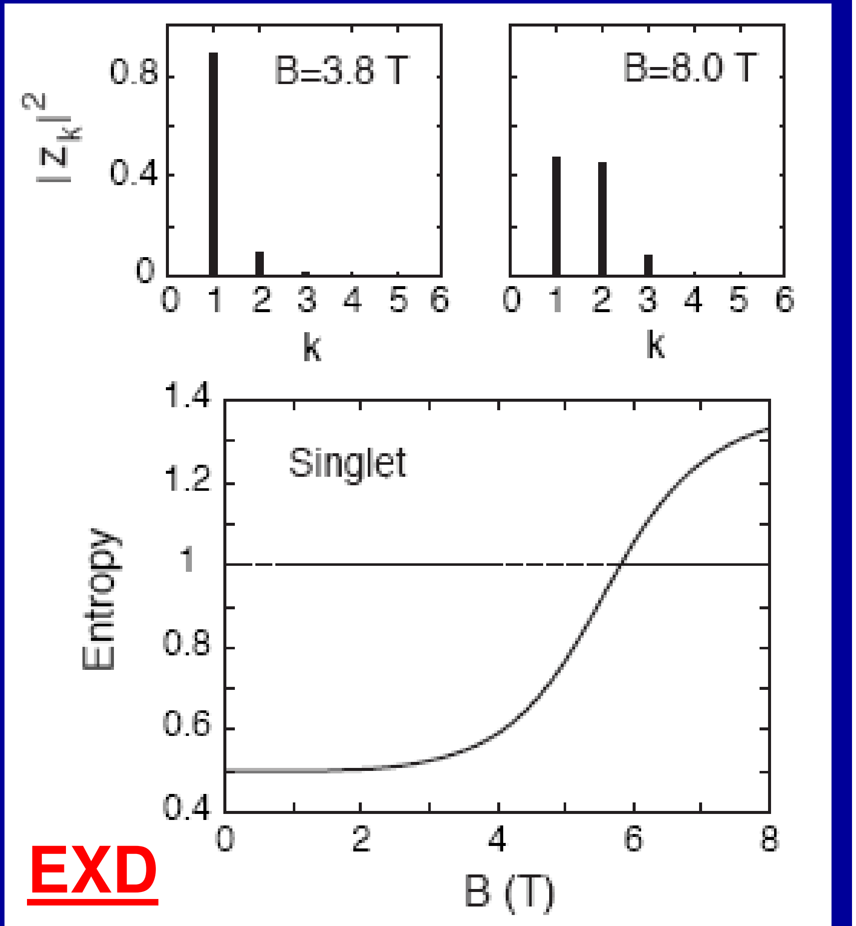
Canonical form:

$$\Psi^{s,t}_{\rm EXD}({\bf r}_1,{\bf r}_2) = \sum_{k=1}^{M} z^{s,t}_k |\Phi(1;2k-1)\Phi(2;2k)\rangle$$

K=79; M <= K

$$\Psi^{s}_{\rm GHL} \propto |\Phi^+(1\uparrow)\Phi^+(2\downarrow)\rangle - \eta|\Phi^-(1\uparrow)\Phi^-(2\downarrow)\rangle$$

$$\Psi^{t}_{\rm GHL} \propto |\Phi^+(1\uparrow)\Phi^-(2\downarrow)\rangle + |\Phi^+(1\downarrow)\Phi^-(2\uparrow)\rangle$$



EXD

ETH single QD

Measure of Entanglement

(Quantum Computing)

Von Neumann Entropy
(indistinguishable parties)

$$S = -\sum_{k=1}^{M} |z_k|^2 \log_2(|z_k|^2)$$

How does one describe entanglement in EXD wfs?

(b) In EXD total spin and its spin projection are good quantum numbers (N, S, S_z)

Spin degeneracies

Branching diagram

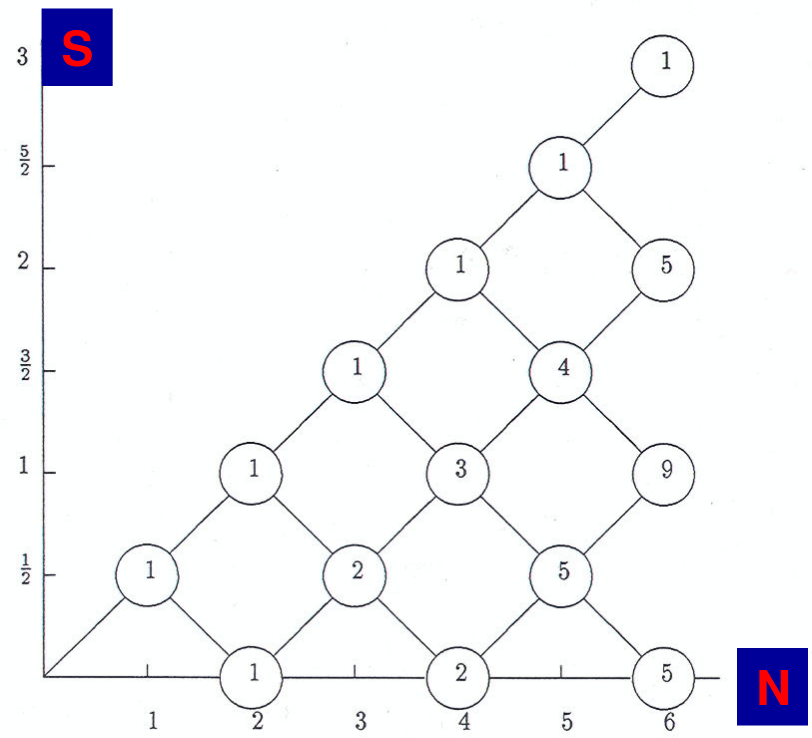


Figure 2.3. Branching diagram.

N-qubit Dicke states

$$|\Psi_{N,k}\rangle = \binom{N}{k}^{-\frac{1}{2}} (|\underbrace{11\ldots1}_{k}000\ldots0\rangle + \text{perm})$$

N-qubit W states

$$|W_N\rangle = |\Psi_{N,1}\rangle$$

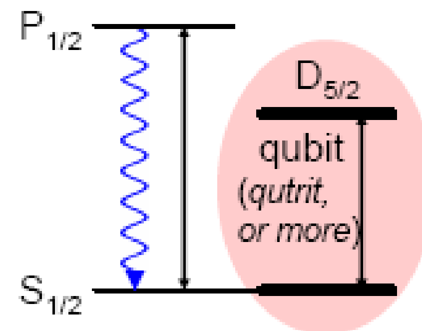
Control and measurement of three-qubit entangled states

C. F. Roos[1], Mark Riebe[1], H. Häffner[1], W. Hänsel[1], J. Benhelm[1], G. P. T. Lancaster[1], C. Becher[1], F. Schmidt-Kaler[1] & R. Blatt[1,2]

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

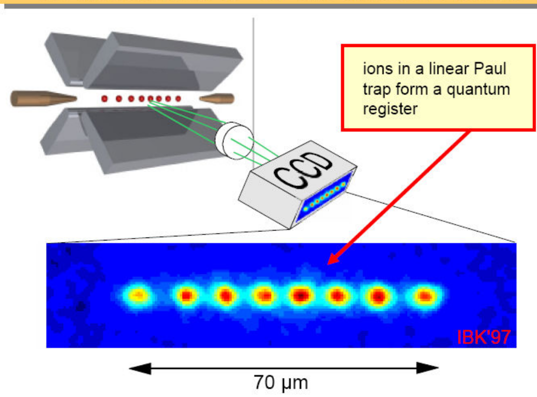
- Basics of ion trap quantum computers
- Entangling operations (Bell states, CNOT)
- Generation of W- and GHZ-states
- Selective read-out of a quantum register
- Entanglement transformation by condional operations

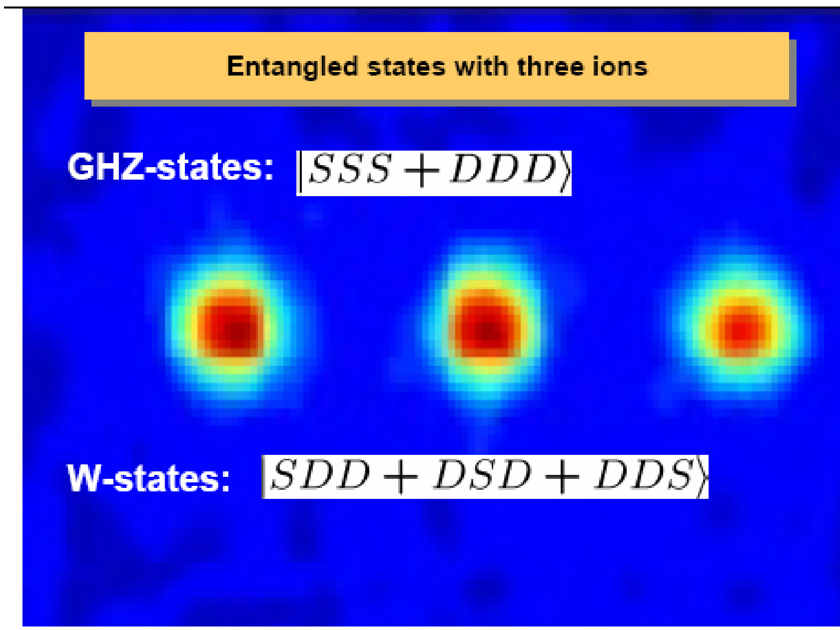
Qubits with trapped ions



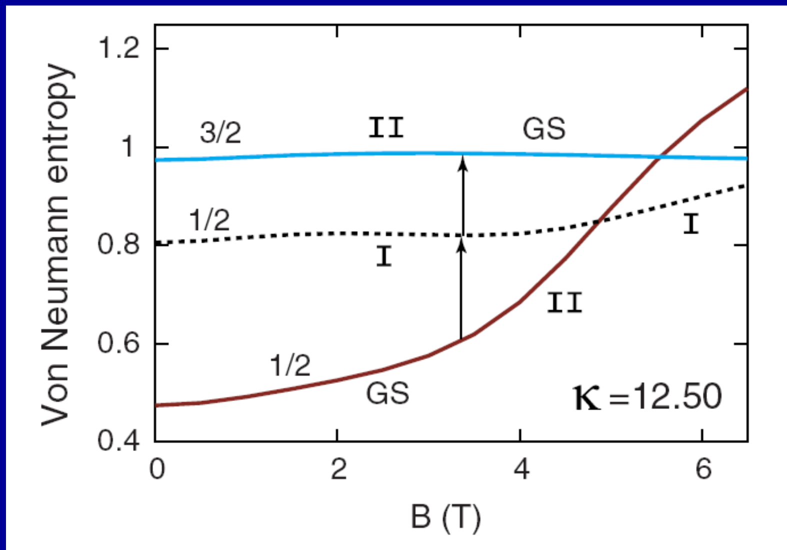
S – D transitions in alkaline earths:
Ca^+, Sr^+, Ba^+, Ra^+, (Yb^+, Hg^+) etc.

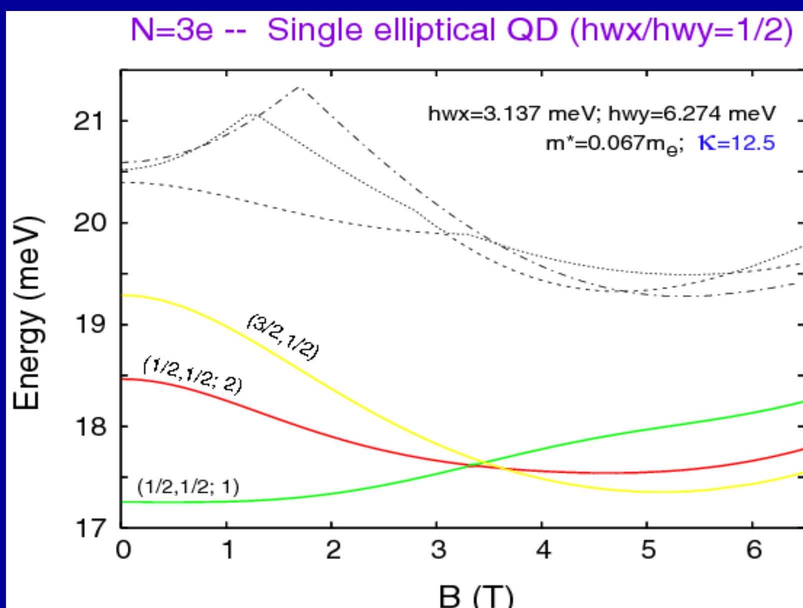
The system: String of $^{40}Ca^+$ ions in a linear Paul trap





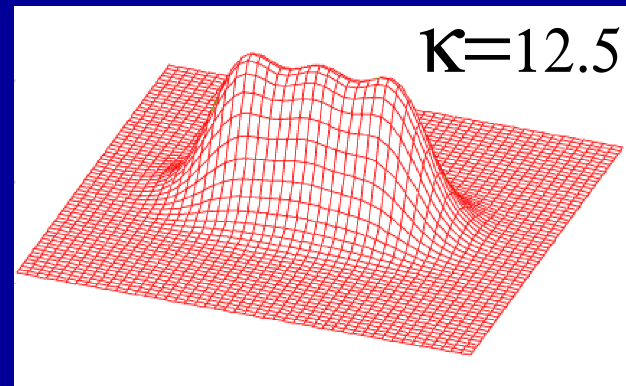
EXD: N=3e in elliptic QD (hwx/hwy=1/2)



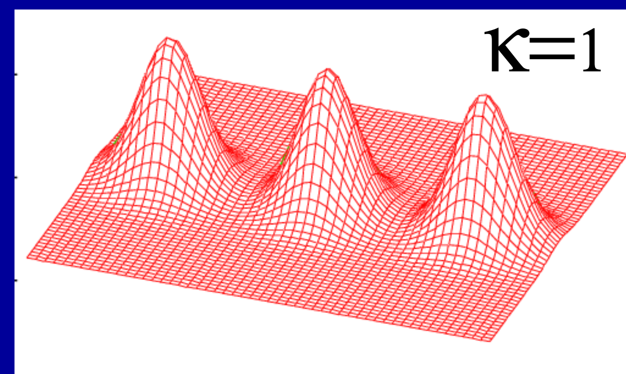


Electron densities

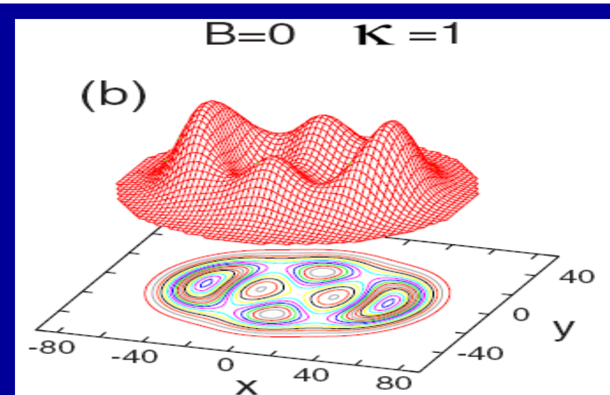
B=0; GS (S=1/2,Sz=1/2)



hwx/hwy=1/2



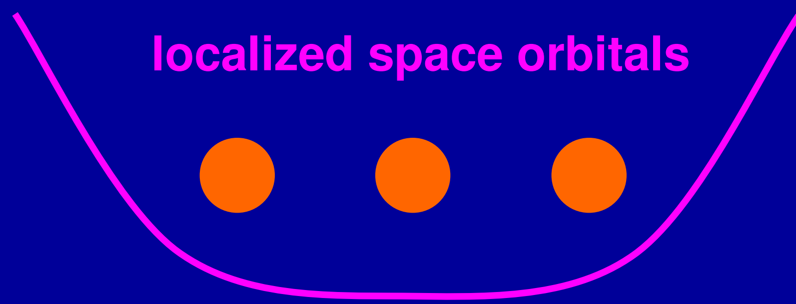
hwx/hwy=1/2



hwx/hwy=0.724

Formation of three-electron Wigner molecule

Elliptic QD

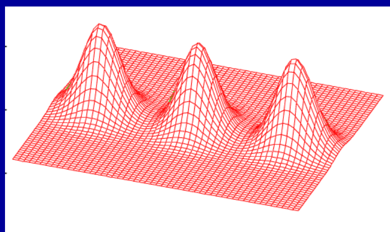


$$\alpha|\uparrow\downarrow\uparrow\rangle+\beta|\downarrow\uparrow\uparrow\rangle+\gamma|\uparrow\uparrow\downarrow\rangle$$

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

(b)



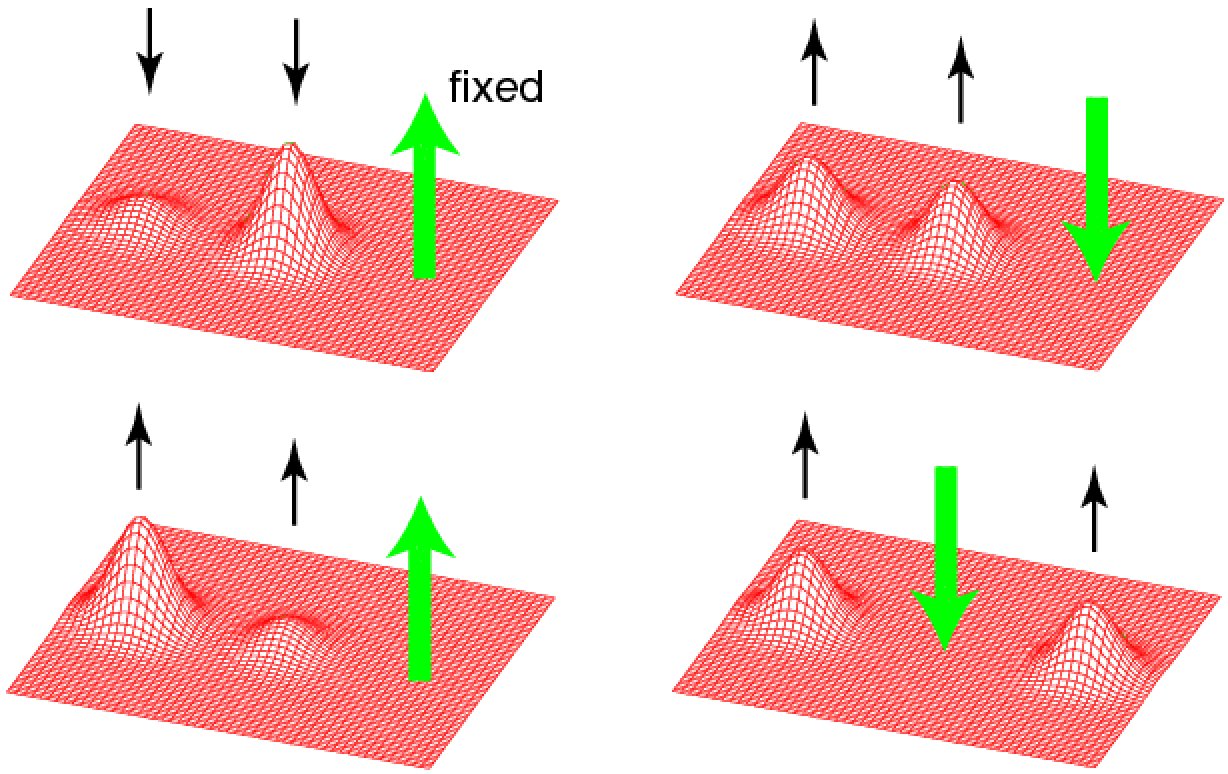
Electron density

Study entanglement by using

Spin resolved CPDs for EXD wfs

Ground-state (1/2,1/2); hwx=3.137 meV; hwx/hwy=1/2;

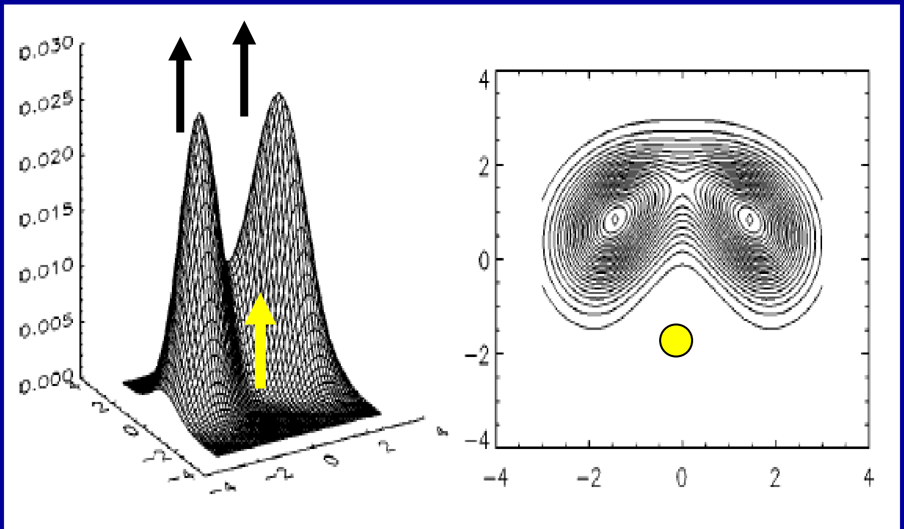
m*=0.067m_e; B=0; κ=1

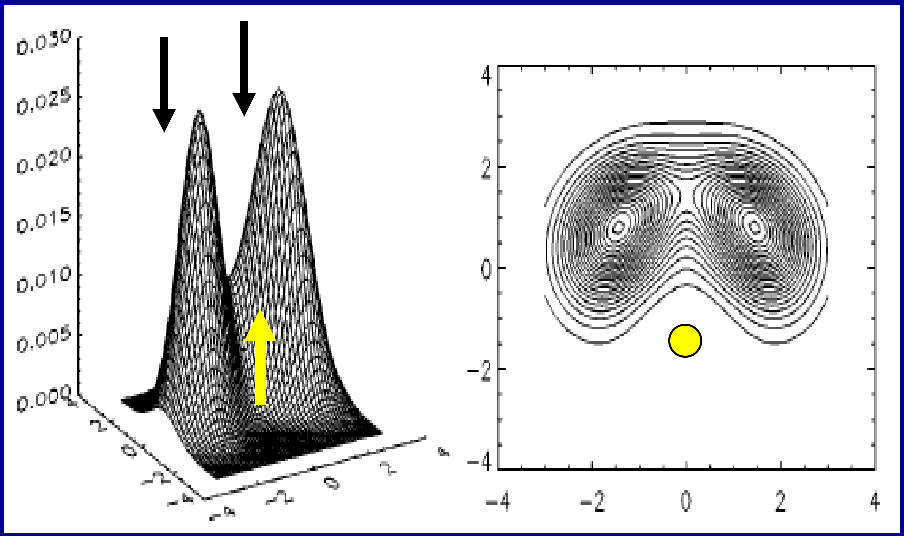


EXD wf $\sim 2|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\rangle$

N=3e; EXD CPDs for Circular dot [S.A. Mikhailov, PRB 65, 115312 (2002)]

L=1; S=1/2, S_z =1/2; R_W = 8





$$\Phi^{E'}_{\rm intr}(\gamma_0) = |\downarrow\uparrow\uparrow\rangle + e^{2\pi i/3}|\uparrow\downarrow\uparrow\rangle + e^{-2\pi i/3}|\uparrow\uparrow\downarrow\rangle$$

$$\Phi^{E''}_{\rm intr}(\gamma_0) = |\downarrow\uparrow\uparrow\rangle + e^{-2\pi i/3}|\uparrow\downarrow\uparrow\rangle + e^{2\pi i/3}|\uparrow\uparrow\downarrow\rangle$$

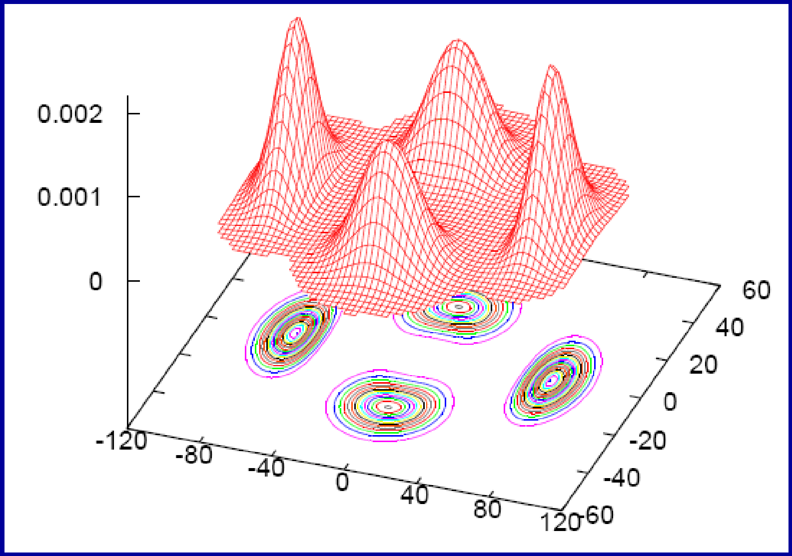
***Intrinsic* wave function ; *rotating* WM; not pinned;**
Cyclic group symmetry

Formation of 4-electron Wigner molecule

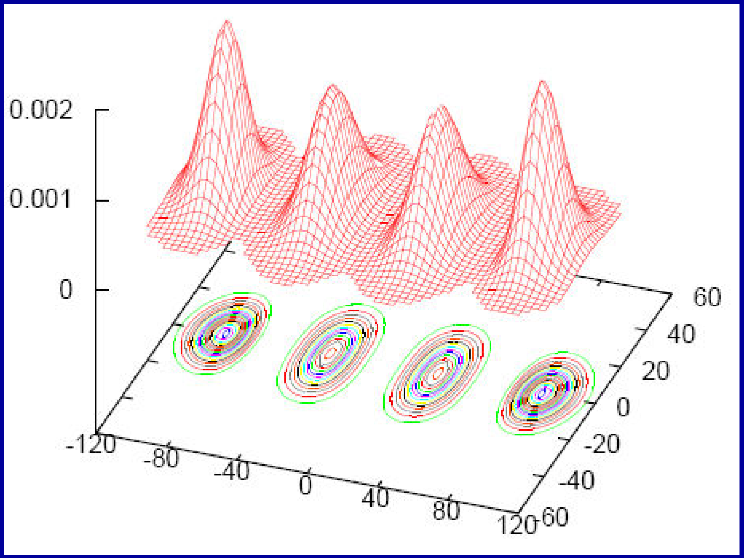
Elliptic QD

(S=1,Sz =1) Lowest energy

*hwx/hwy =**1/2***



*hwx/hwy =**1/3***



hwx=3.14 meV

hwy=6.28 meV

κ=0.60

B=0

hwx=2.24 meV

hwy=6.71 meV

General spin function for a (S=0,Sz =0) state with N=4 localized electrons

$$\chi_{00}(\theta) = \sqrt{\frac{1}{3}}\sin\theta|\uparrow\uparrow\downarrow\downarrow\rangle + \left(\frac{1}{2}\cos\theta - \sqrt{\frac{1}{12}}\sin\theta\right)|\uparrow\downarrow\uparrow\downarrow\rangle - \left(\frac{1}{2}\cos\theta + \sqrt{\frac{1}{12}}\sin\theta\right)|\uparrow\downarrow\downarrow\uparrow\rangle$$
$$- \left(\frac{1}{2}\cos\theta + \sqrt{\frac{1}{12}}\sin\theta\right)|\downarrow\uparrow\uparrow\downarrow\rangle + \left(\frac{1}{2}\cos\theta - \sqrt{\frac{1}{12}}\sin\theta\right)|\downarrow\uparrow\downarrow\uparrow\rangle + \sqrt{\frac{1}{3}}\sin\theta|\downarrow\downarrow\uparrow\uparrow\rangle$$

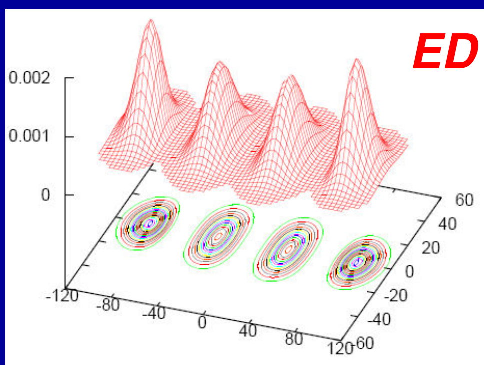
(in book by K. Varga)

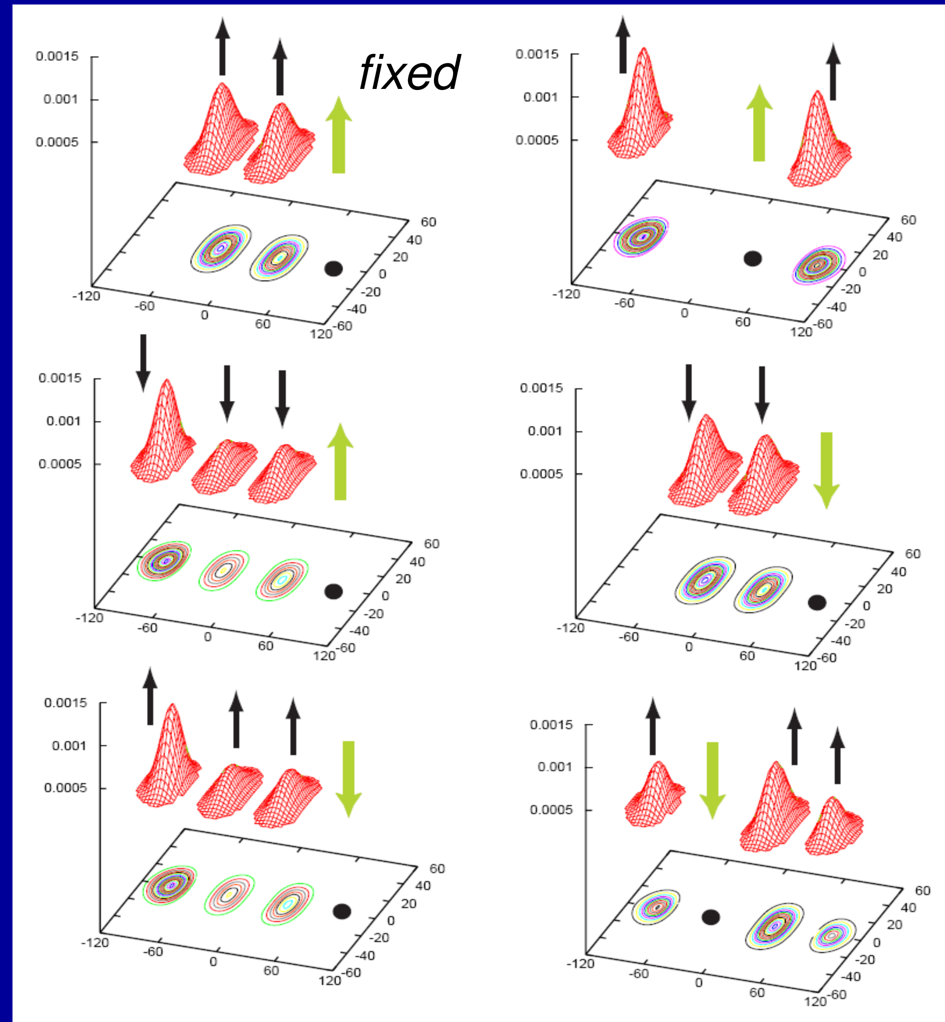
Can this spin function be properly characterized as antiferromagnetic?

It is a multideterminantal wf!
It expresses entanglement!
(non-symmetric Dicke state!)

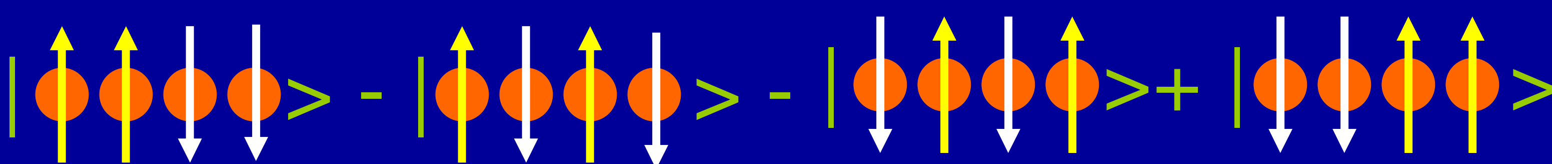
Spin resolved CPDs for N=4
(second case in previous slide: anisotropy=1/3)

(S=0,Sz =0)
Second lowest energy with these quantum numbers





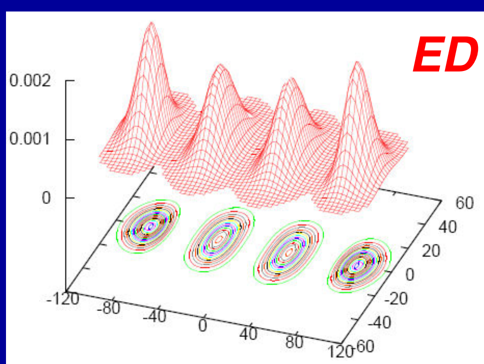
EXD wf $(\theta = 120^o)$ ~

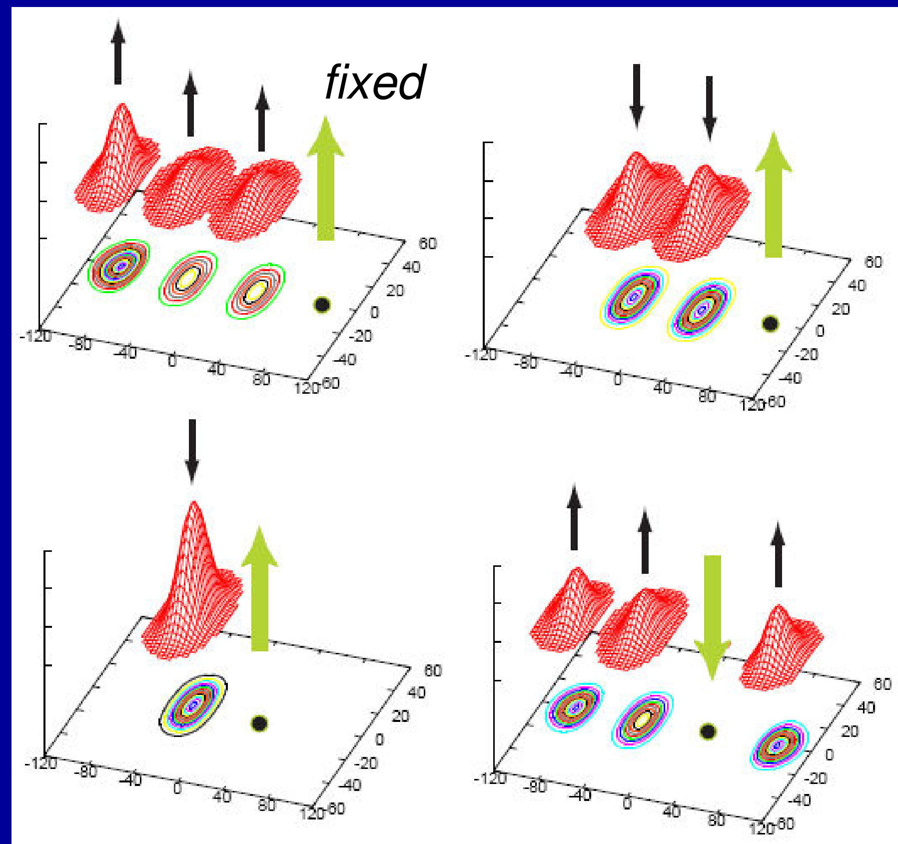


Dicke state

Spin resolved CPDs for N=4 (anisotropy=1/3)

(S=1,Sz =1) Lowest energy with these quantum numbers





EXD wf ~ |↑↑↓↑> - |↑↓↑↑>

W state

SUMMARY (first part)

Few electrons in an elliptic QD can form for large anisotropies
linear Wigner molecules

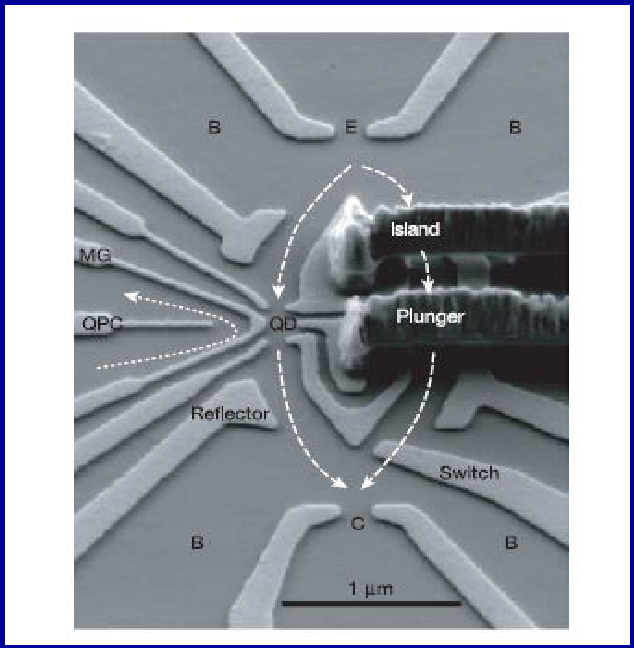
The many-body EXD wave functions in the
linear Wigner Molecule regime are related to
entangled W and Dicke states

Using the EXD wave function, one can determine the
degree of entanglement of few indistinguishable electrons
in a quantum dot

Exact-diagonalization treatment of the non-universal transport regime in few-electron quantum dots

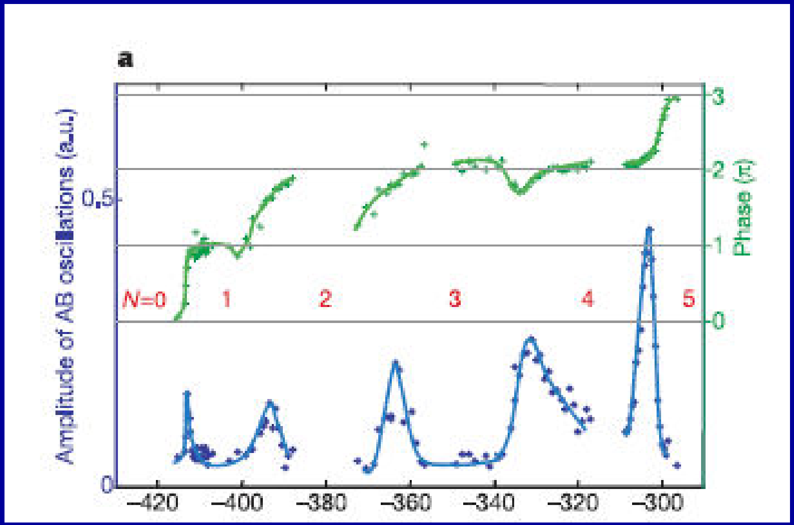
Leslie O. Baksmaty, Constantine Yannouleas, Uzi Landman
School of Physics, Georgia Institute of Technology

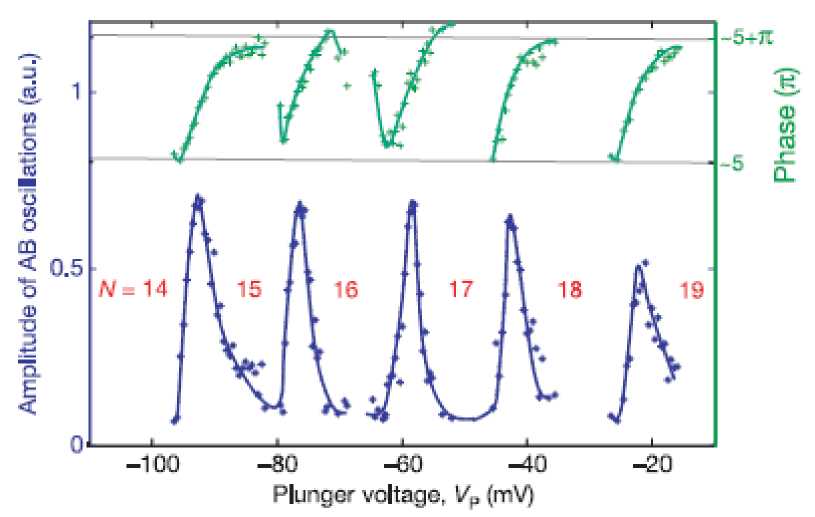
Phys. Rev. Lett. 101, 136803 (2008)



Experiment:
M. Avinun-Kalish et al.,
Nature **436**, 529 (2005)

Experiment: Aharonov-Bohm interferometry:
M. Avinun-Kalish et al., Nature **436**, 529 (2005)





Non-universal regime

Universal regime

It is essential to have the best description for the QD electronic structure

EXD -> Full CI (superposition of single-particle configurations ~ 100,000),
see e.g. Yannouleas and Landman, Rep. Prog. Phys. **70**, 2067 (2007)

Non-universal regime:
Current and transmission phase depend strongly on the details and electronic structure (many-body problem) of the quantum dot .
They vary slowly with the tunneling coupling in a given experimental setup.

Transport approach

Weak tunneling coupling: Lowest order in coupling – Golden rule

- John Bardeen's seminal paper: "Tunneling from a many-body point of view" PRL **6**, 57 (1961) -- Current

- J.M. Kinaret et al., PRB **46**, 4681 (1992) -- Current

- For transmission phase: S.A. Gurvitz, PRB **77**, 201302 (2008) (only first half of paper)

$$H = H_L + H_R + H_D + H_T$$

$$H_T = \left(\sum_{l,k} \Omega_l^{(k)} d_k^\dagger a_l + l \leftrightarrow r \right) + H.c.$$

$$\Omega_{l(r)}^{(k)} = -\frac{\hbar^2}{2m} \int_{\boldsymbol{x} \in \Sigma_{l(r)}} \phi_k(\boldsymbol{x}) \overleftrightarrow{\nabla} \boldsymbol{n} \; \chi_{l(r)}(\boldsymbol{x}) d\sigma$$

Tails under a tall barrier

Quasiparticle in QD

Leads: non-interacting

Previous calculations:

QD described with independent-particle model

(Hackenbroich et al, PRL 76, 110 (1996))

This study: Electronic structure of QD described through exact diagonalization (EXD; includes e-e correlations)

EXD quasiparticle wave function

$$\Phi_N^{\rm EXD}(S,S_z;k) = \sum_I C_I^N(S,S_z;k) D^N(I;S_z)$$

$$\mathcal{H} = \sum_{i=1}^N [\mathbf{p}_i^2/(2m^*) + V(x_i,y_i)] + \sum_{i<j} e^2/(\kappa r_{ij})$$

$$V(x,y) = m^*(\omega_x^2 x^2 + \omega_y^2 y^2)/2$$

$$\varphi_{\rm QP}(\mathbf{r}) = \langle \Phi_{N-1}^{\rm EXD} | \psi(\mathbf{r};\sigma) | \Phi_N^{\rm EXD} \rangle$$

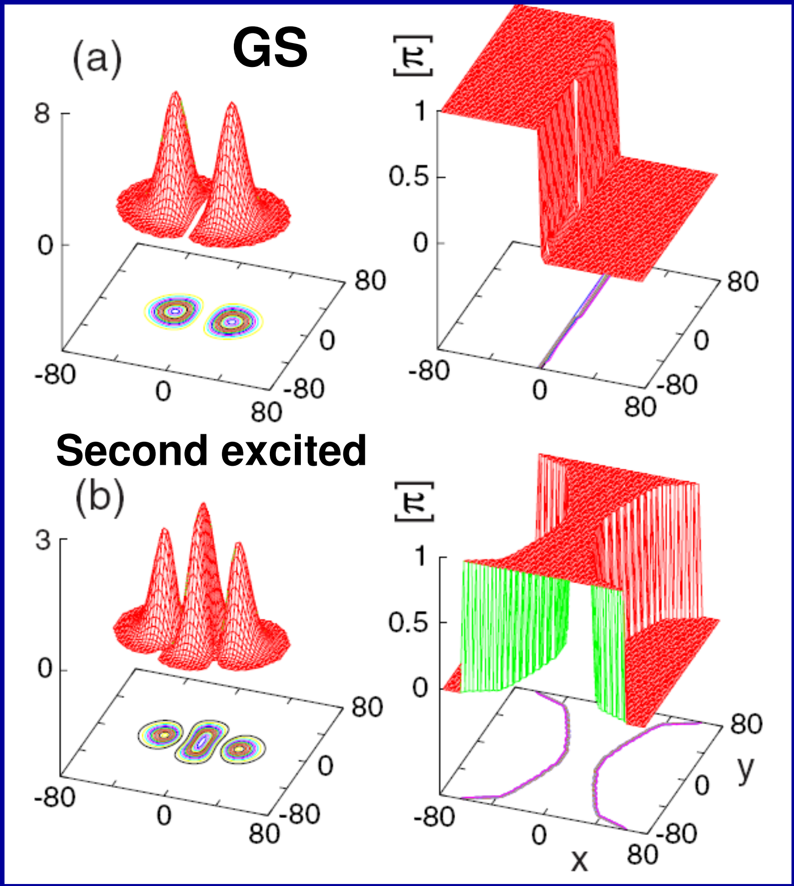
$$\psi(\mathbf{r};\sigma) = \sum_{i=1}^K \phi_i(\mathbf{r}) a_i(\sigma)$$

$$\varphi_{\rm QP}(\mathbf{r})$$

eta=0.724
kappa=12.5

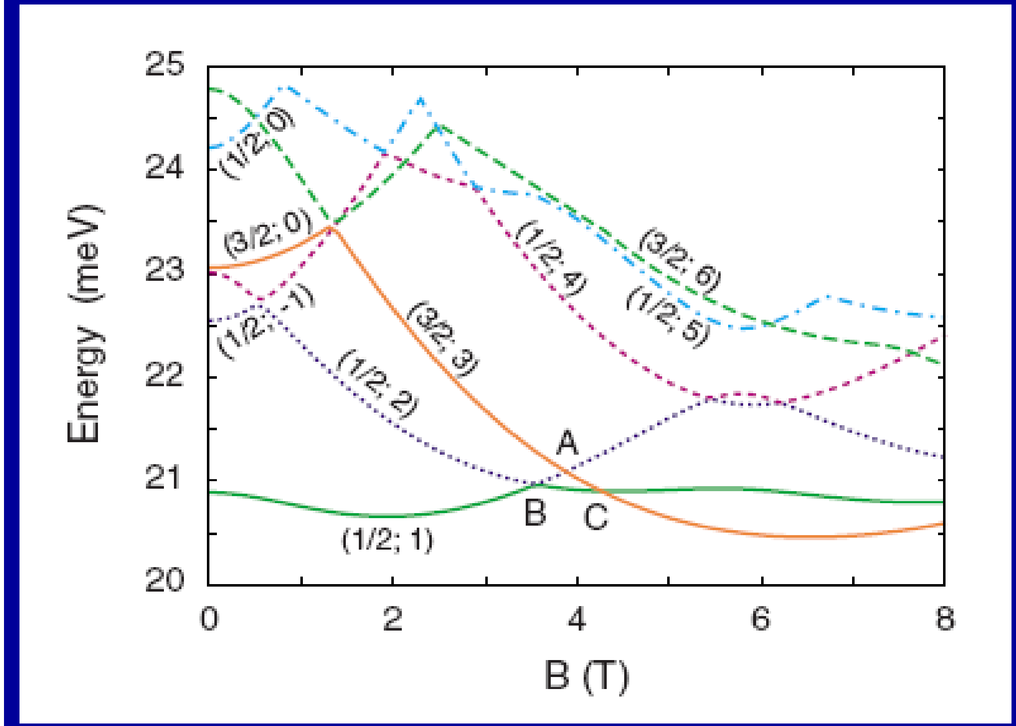
amplitude (modulus square)

transmission phase



(0,0) N=2 → N=3 (1/2,1/2)

EXD quasiparticle wave function



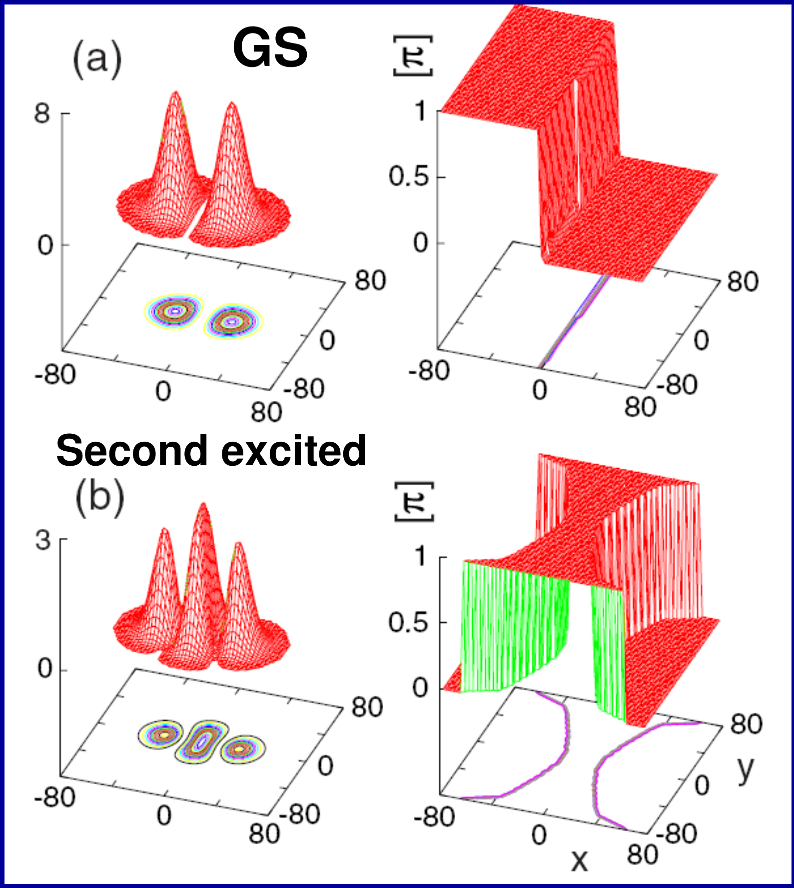
$$\varphi_{\rm QP}(\mathbf{r}) = \langle \Phi_{N-1}^{\rm EXD} | \psi(\mathbf{r};\sigma) | \Phi_N^{\rm EXD} \rangle$$

$$\psi(\mathbf{r};\sigma) = \sum_{i=1}^{K} \phi_i(\mathbf{r}) a_i(\sigma)$$

$$\varphi_{\rm QP}(\mathbf{r})$$

eta=0.724
kappa=12.5

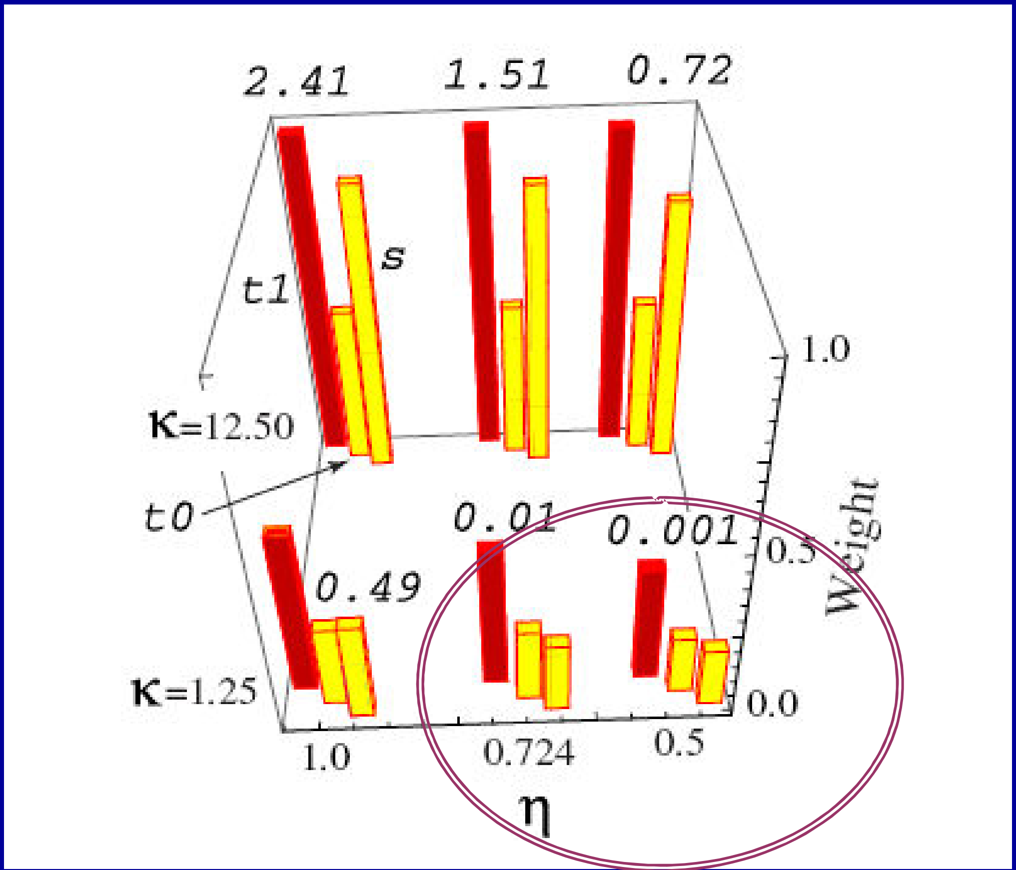
amplitude (modulus square) **transmission phase**



(0,0) N=2 → N=3 (1/2,1/2)

Bar-chart: N =1 → N=2

$$\mathcal{W} = \int |\varphi_{\mathrm{QP}}(\mathbf{r})|^2 d\mathbf{r}$$



Doorway excited states

θ_{QP} → Red → π ; Yellow → 0

$\theta = \theta_{\mathrm{QP}} - \pi$ → **(No PL)** √ ; **(Yes PL)**

Strength of e-e interaction:

Dielectric constant κ

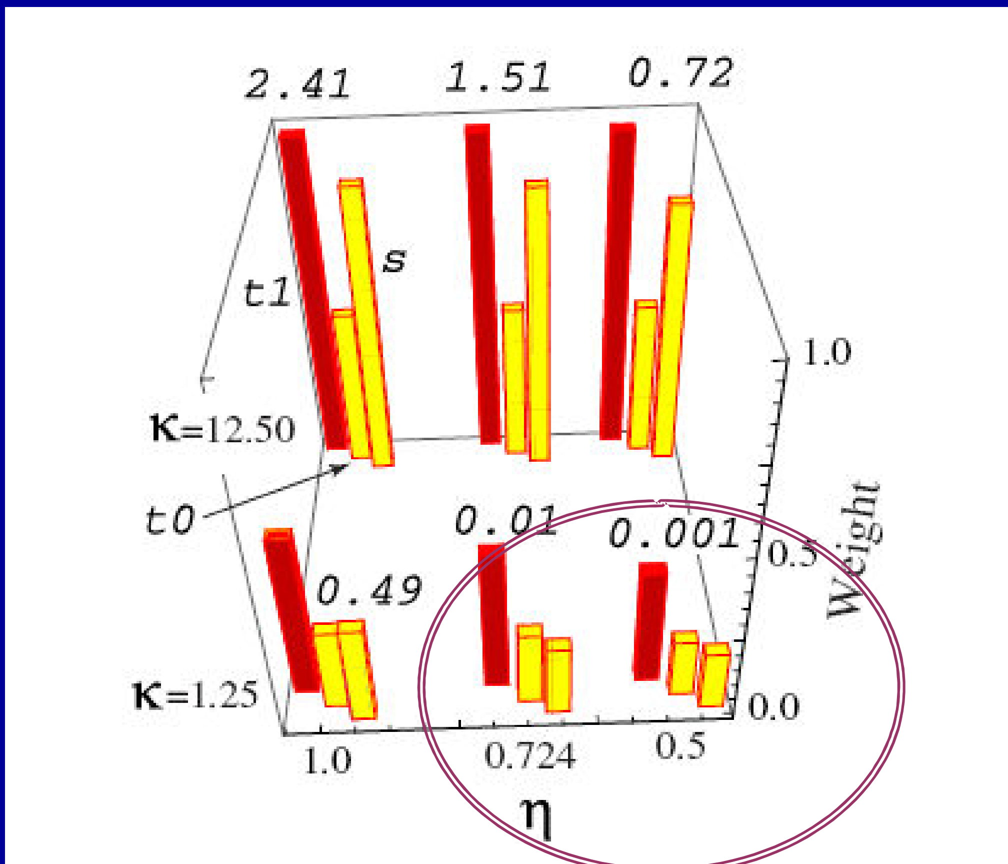
Anisotropy: $\eta = \omega_x / \omega_y$

$\omega_0 = \sqrt{(\omega_x^2 + \omega_y^2)/2}$

$\hbar\omega_0$ = 5 meV

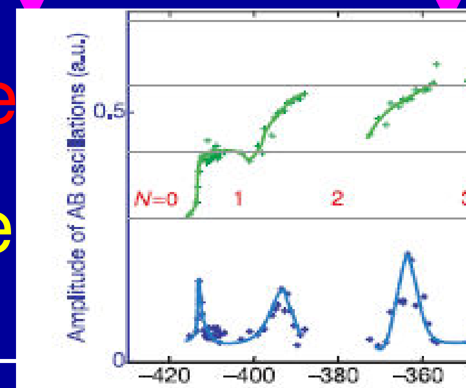
Bar-chart: N =1 → N=2

$$\mathcal{W} = \int |\varphi_{\rm QP}(\mathbf{r})|^2 d\mathbf{r}$$



$$\theta_{\rm QP}$$

$$\theta = \theta_{\rm QP} - \pi$$



Re PL) √

Ye s PL)

Strength of e-e interaction:

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$\hbar\omega_0$ = 5 meV

Doorway excited states

Spin configurations for a 3e QD treated with EXD

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

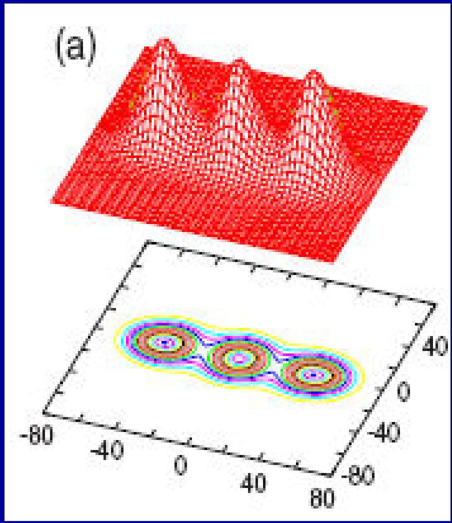
(S, S_z)

$$\Phi\left(\tfrac{3}{2},\tfrac{3}{2}\right) = |\uparrow\uparrow\uparrow\rangle$$

$$\sqrt{3}\,\Phi\left(\tfrac{3}{2},\tfrac{1}{2}\right) = |\uparrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\uparrow\rangle$$

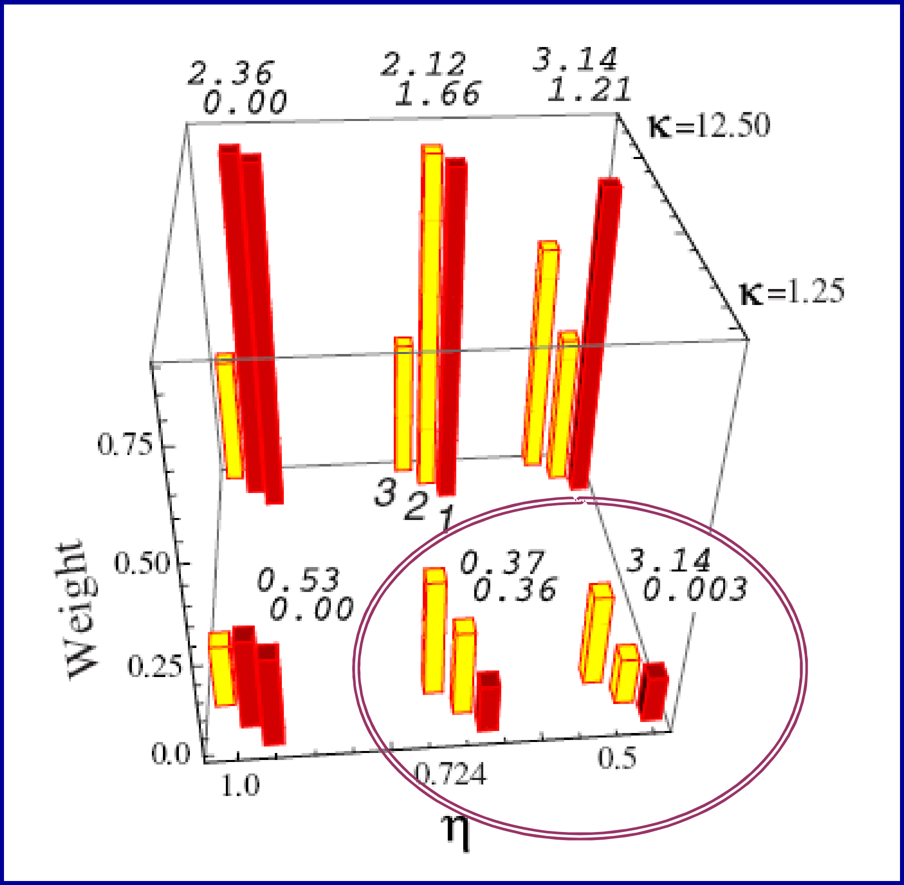
$$\sqrt{6}\,\Phi\left(\tfrac{1}{2},\tfrac{1}{2};1\right) = 2|\uparrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle$$

$$\sqrt{2}\,\Phi\left(\tfrac{1}{2},\tfrac{1}{2};2\right) = |\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle$$



Bar-chart: N =2 → N=3 [(0,0) → (1/2,1/2)]

$$\mathcal{W} = \int |\varphi_{\mathrm{QP}}(\mathbf{r})|^2 d\mathbf{r}$$



θ_{QP} ↓ Red → π

$\theta = \theta_{\mathrm{QP}} - \pi$ ↓ (No PL)

Yellow → 0 (Yes PL) √

Strength of e-e interaction:

Dielectric constant κ

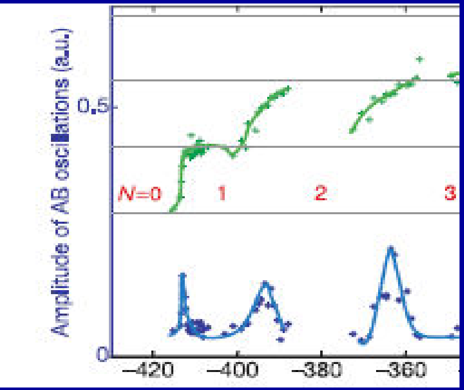
Anisotropy: $\eta = \omega_x / \omega_y$

Doorway excited states

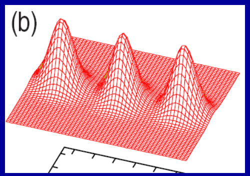
Conclusions (second part)

- Non-universal regime of electron interferometry can be described using Bardeen's weak-coupling theory and exact diagonalization for QD

- We find (in agreement with experiment): →
  a) for N=1 → N=2: no phase lapse
  b) for N=2 → N=3: phase lapse of π



- Agreement for QDs with anisotropy and strong e-e repulsion, favoring regime of Wigner molecule formation →



- Importance of doorway excited states and many-body spin configurations