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

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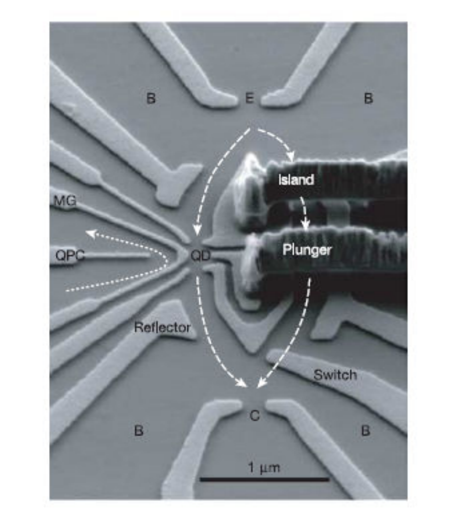


Experiment:
M. Avinun-Kalish et al., Nature **43**6, 529 (2005)

APS March 2008

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, arXiv: 0704:1260

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

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

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

Tails under a tall barrier

Quasiparticle in QD

Leads: non-interacting

Previous calculations:

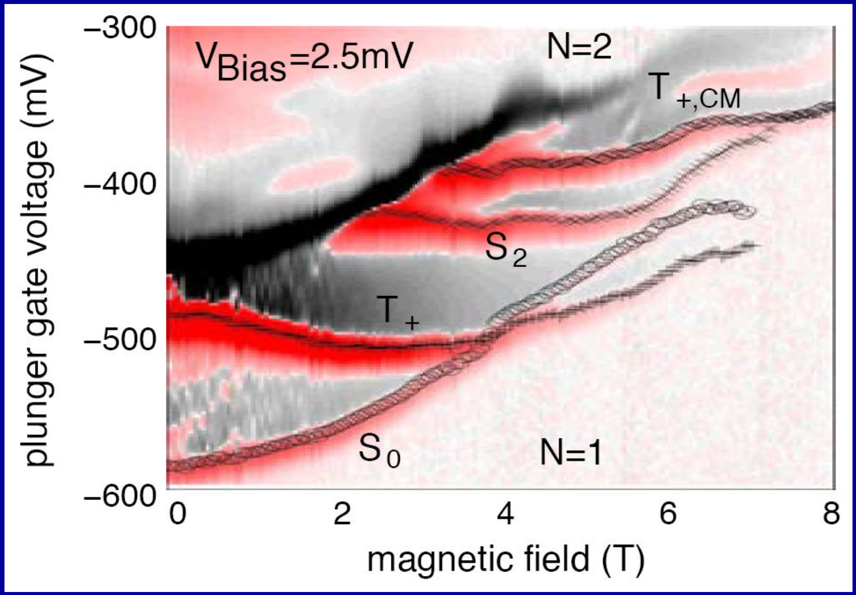
QD described with independent-particle model

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

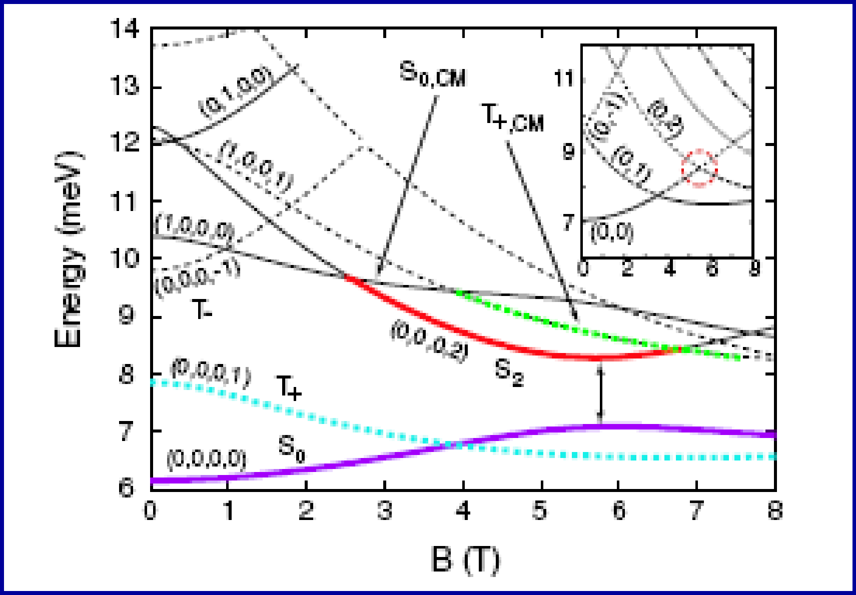
This study: Electronic structure of QD described through exact diagonalization (EXD; includes e-e correlations)

IMPORTANCE OF EXD: N=2 electron anisotropic QD

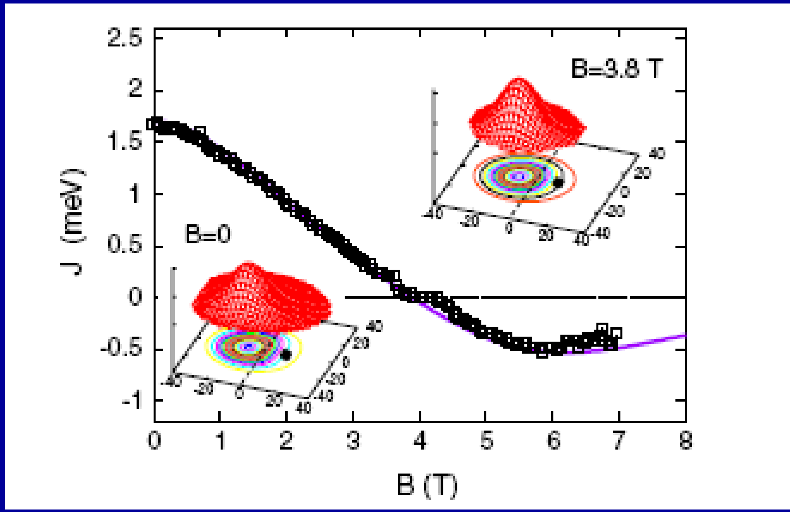
Experiment



Theory (EXD)

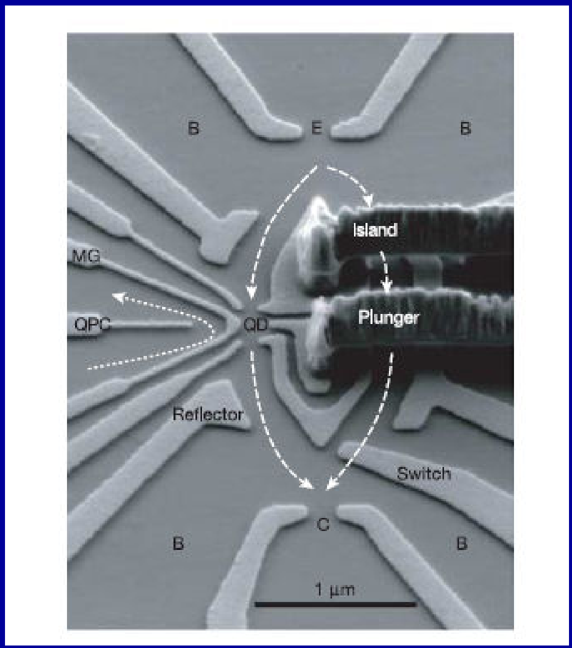


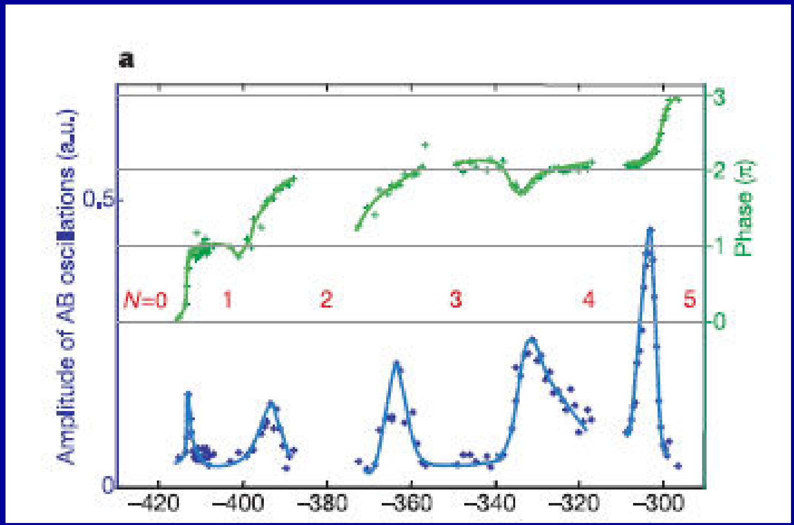
[Ellenberger et al, PRL **96**, 126806 (2006)]



Strong correlations:
Wigner molecules

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





N<15: Non-universal (mesoscopic) 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)

For the latest developments of EXD concerning 3e anisotropic QDs:
Yuesong Li et al, PRB **76,** 245310 (2007)

EXD quasiparticle wave function

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

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

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

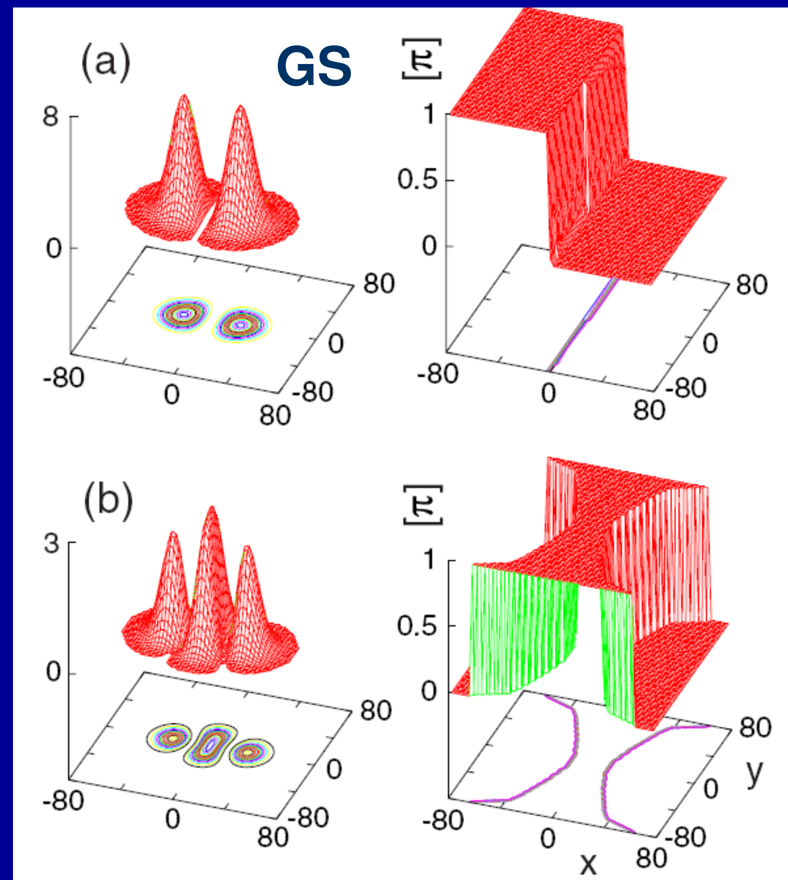
$$\varphi_{\mathrm{QP}}(\mathbf{r}) = \langle \Phi_{N-1}^{\mathrm{EXD}} | \psi(\mathbf{r}; \sigma) | \Phi_N^{\mathrm{EXD}} \rangle$$

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

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

amplitude (modulus square)

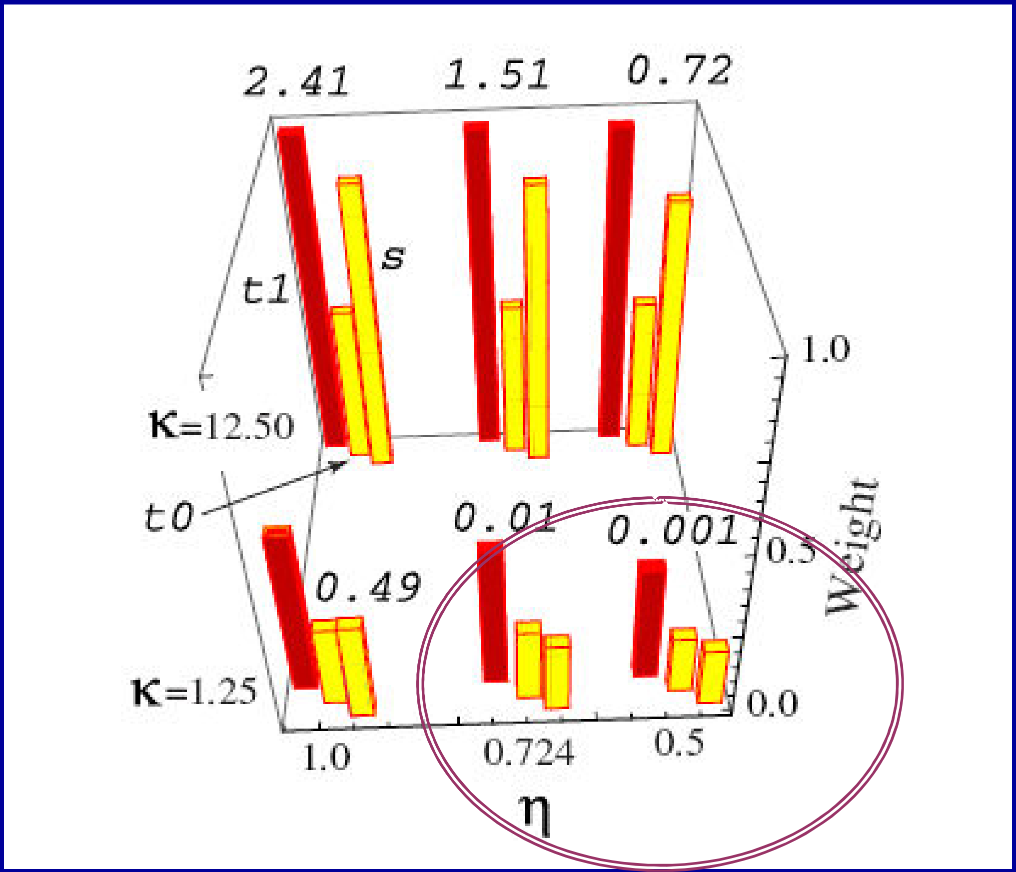
transmission phase



(0,0) N=2 → N=3 (1/2,1/2)

Bar-chart: N =1 → N=2

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



Doorway excited states

$\theta_{\rm QP}$ → Red → π

$\theta = \theta_{\rm QP} - \pi$ → (No PL) √

Yellow → 0 (Yes PL)

Strength of e-e interaction:

Dielectric constant κ

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

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

$\hbar\omega_0$ = 5 meV

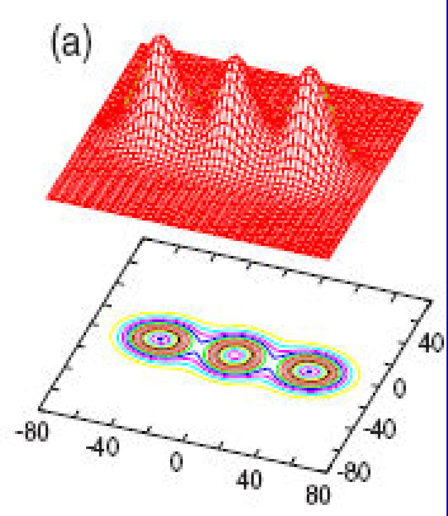
Spin configurations for a 3e QD treated with EXD

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

(S, S_z)

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

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

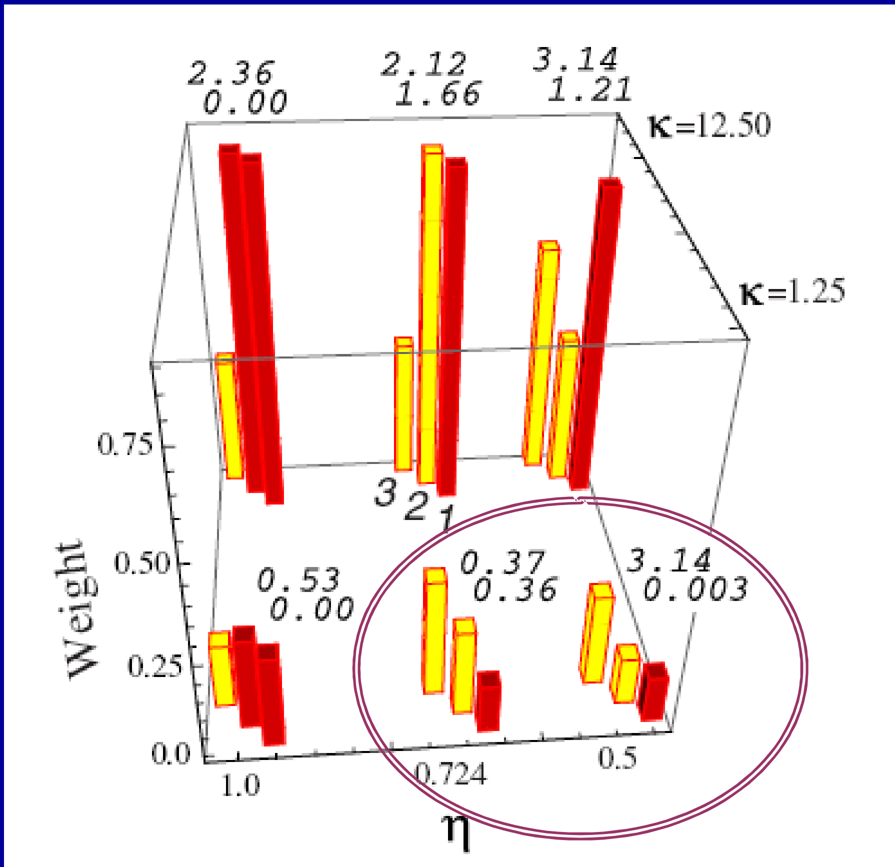


$$\sqrt{6}\Phi\left(\tfrac{1}{2},\tfrac{1}{2};1\right) = 2|\uparrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle$$

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

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 ; Yellow → 0

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

Red → π (No PL)

Yellow → 0 (Yes PL) √

Strength of e-e interaction:

Dielectric constant κ

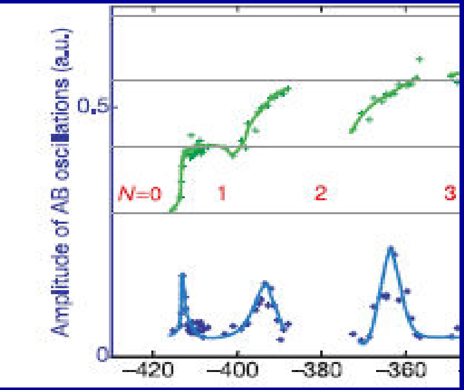
Anisotropy: $\eta = \omega_y / \omega_x$

Doorway excited states

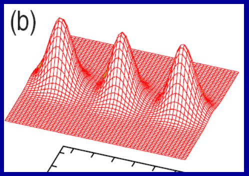
Conclusions

- 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