Strong Correlations in Quantum Dots and Wires: Quantum Monte Carlo Studies

Harold U. Baranger, *Duke University*

Tunable electron-electron correlation in nanosystems:

1. **Strong interactions:** low density → strong interactions
2. **Dimensionality:** 1D → particles can't pass → interact
3. **Charging:** energy required to place additional electron

Two examples:

I. Quantum phase transition and dynamically enhanced symmetry in 4 quantum dots

- correlation of localized electron coupled to electron gas

II. Interaction-induced localization in a quantum wire

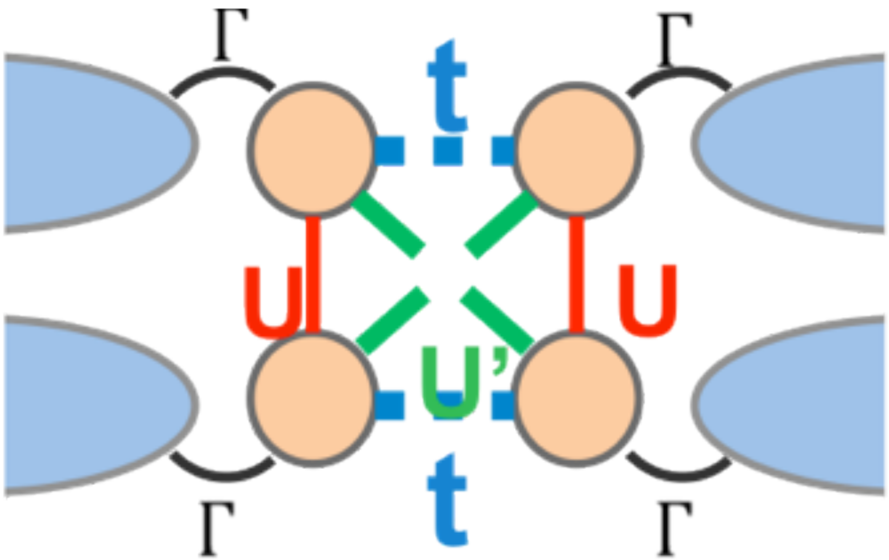
- tune density by gate + quasi-1D → localization
- barriers form dynamically → Coulumb blockade physics

Quantum Phase Transition and Dynamically Enhanced Symmetry in Quadruple Quantum Dot System

(Dong Liu, S. Chandrasekharan, HUB)

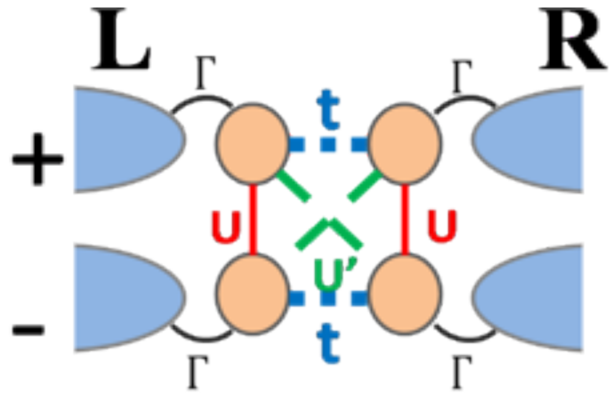
Motivation:

1. **3 competing interactions**: Kondo, Heisenberg, Ising
   ➔ 2 dimensionless parameters that can be tuned
2. Probe **boundary QPT** and Kondo-like **enhancement of symmetry** in nano-system; potentially realizable in experiment.
3. (Develop Quantum Monte Carlo code for complex impurity systems.)



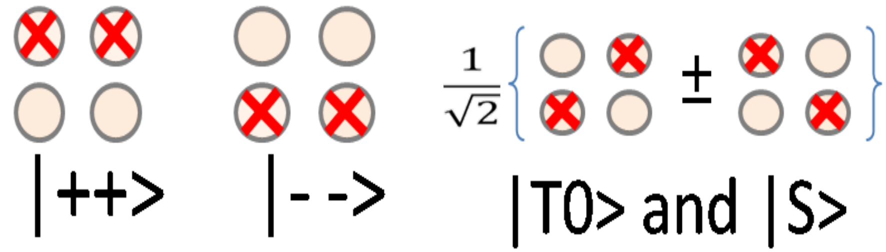
Single level on each dot,
2 spinless electrons,
capacitively coupled

Model: 4 Quantum Dots



2 electrons in the 4 dots & U≫U'

➔ Eigenstates of the impurity:



$$H = H_{lead} + H_{imp} + H_{coupling}$$

$$H_{imp} = \sum_{i}^{L,R}\left(\sum_{s}^{+,-}\varepsilon_{is}d_{is}^{+}d_{is} + Un_{i+}n_{i-}\right) + U'\left(n_{L+}n_{R-} + n_{L-}n_{R+}\right) + t\sum_{s}^{+,-}\left(d_{Ls}^{+}d_{Rs} + d_{Rs}^{+}d_{Ls}\right)$$

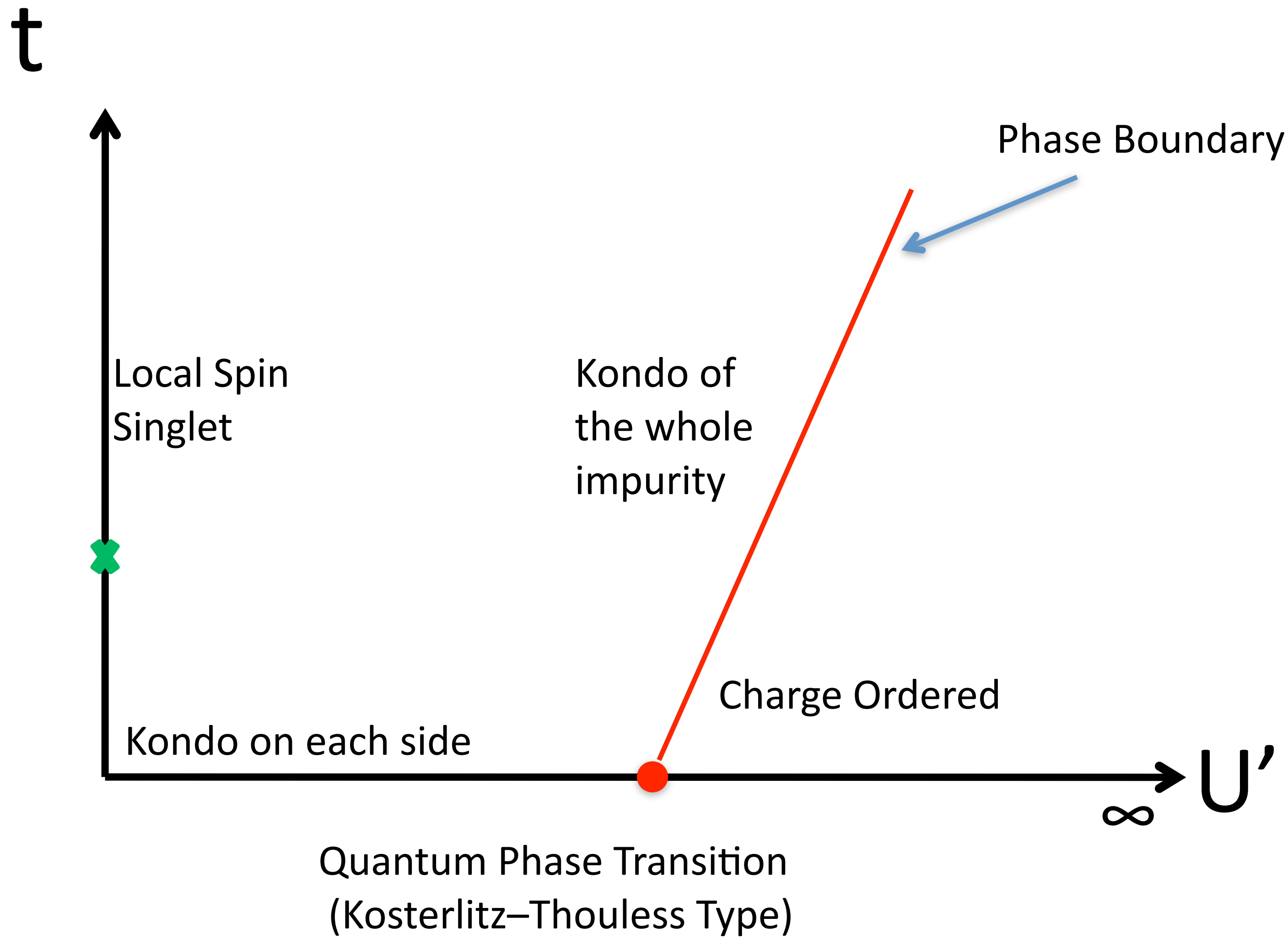
For t≪U, Anderson➔Kondo: $\boxed{H_{imp}^{eff} \approx J\,\overrightarrow{S_L}\cdot\overrightarrow{S_R} - \tilde{J}_z\,S_L^z S_R^z}$

Pseudospin $\vec{S}_L \equiv \frac{1}{2}\sum_{s,s'}^{+,-} d_{Ls}^{\dagger}\vec{\sigma}_{s,s'}d_{Ls'}$ $\quad J \sim \frac{t^2}{U} \quad \tilde{J}_z \sim U'$

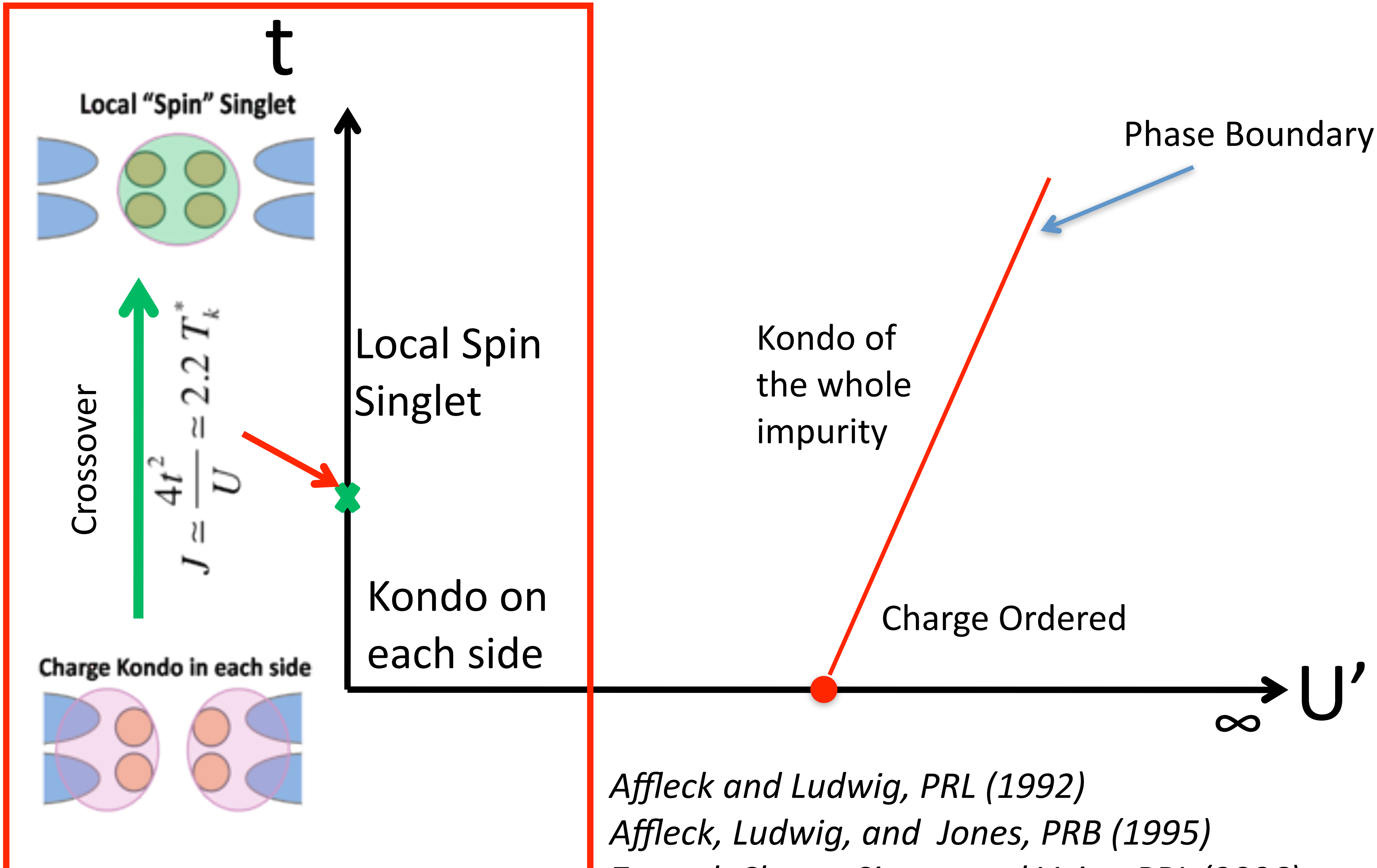
tunable

Ground State Phase Diagram

$t/U \ll 1$



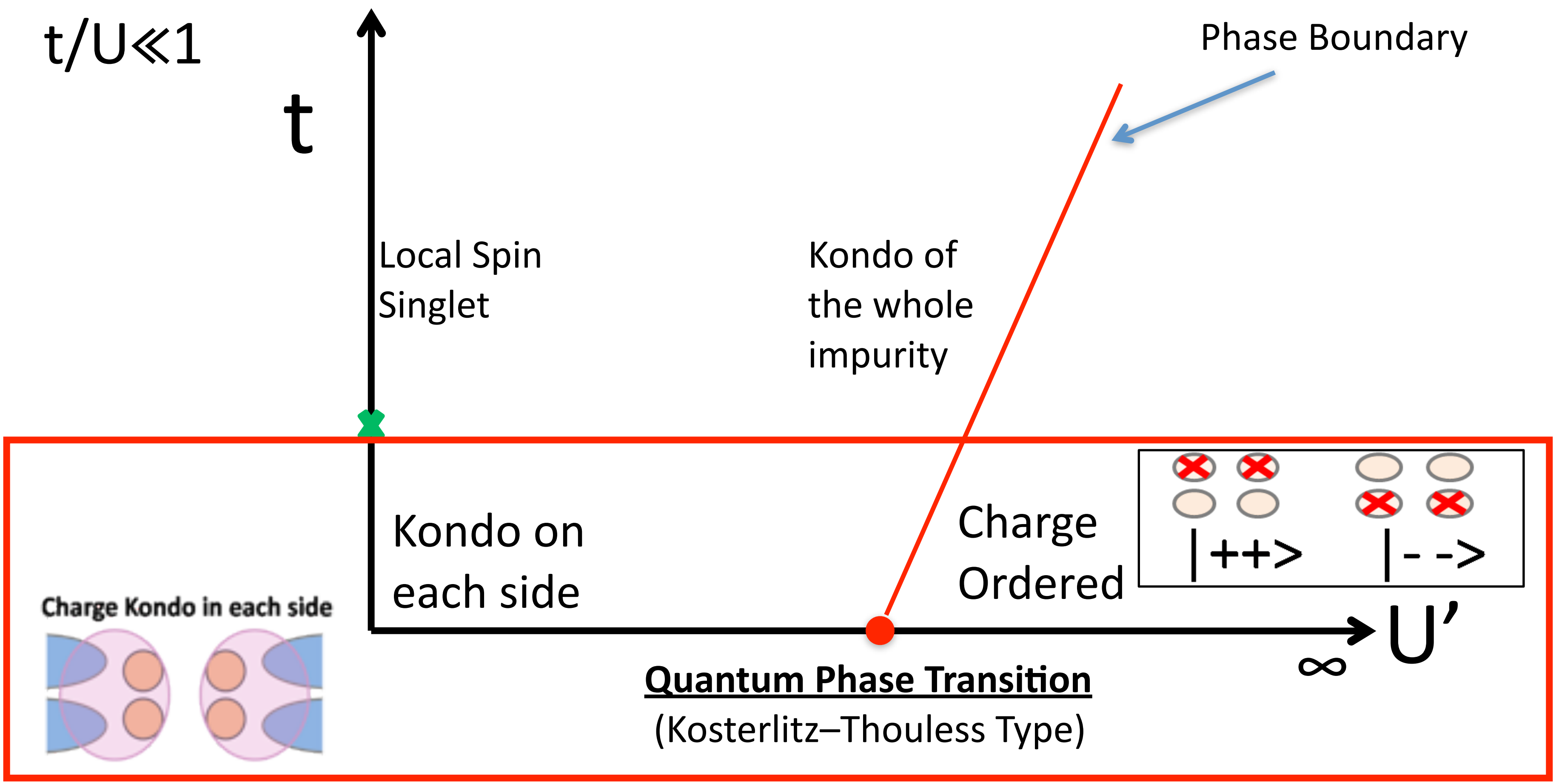
Ground State Phase Diagram



t/U≪1

Affleck and Ludwig, PRL (1992)
Affleck, Ludwig, and Jones, PRB (1995)
Zarand, Chung, Simon, and Vojta, PRL (2006)
Experiment in double quantum dots:
A. M. Chang group, Science (2001)

Ground State Phase Diagram

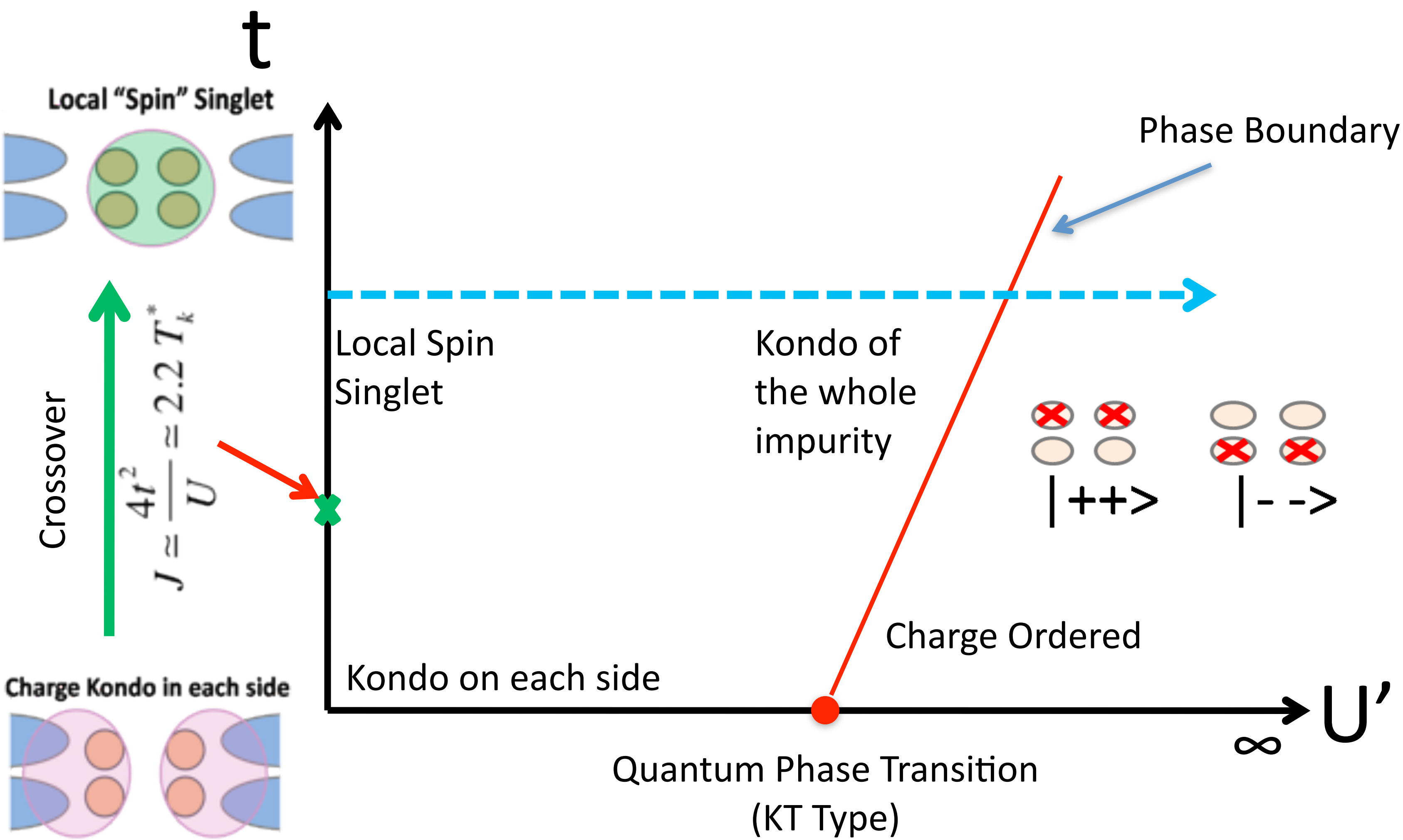


Garst, Kehrein, Pruschke, Rosch, Vojta; PRB (2004)
Galpin, Logan, Krishnamurthy; PRL (2005) & J. Phys. CM (2006)

NO EXPERIMENT (YET!)

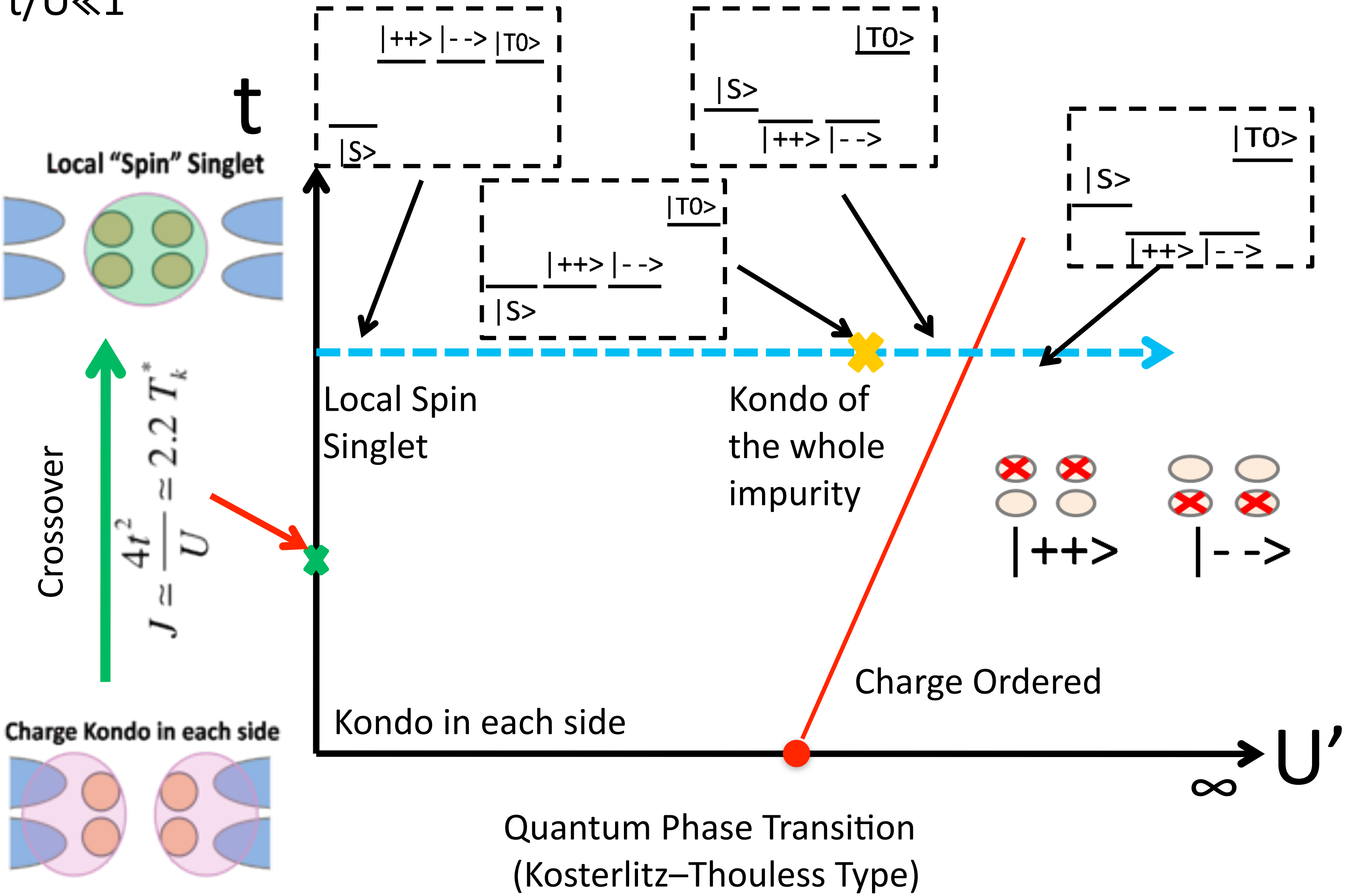
Ground State Phase Diagram

$t/U \ll 1$



Ground State Phase Diagram

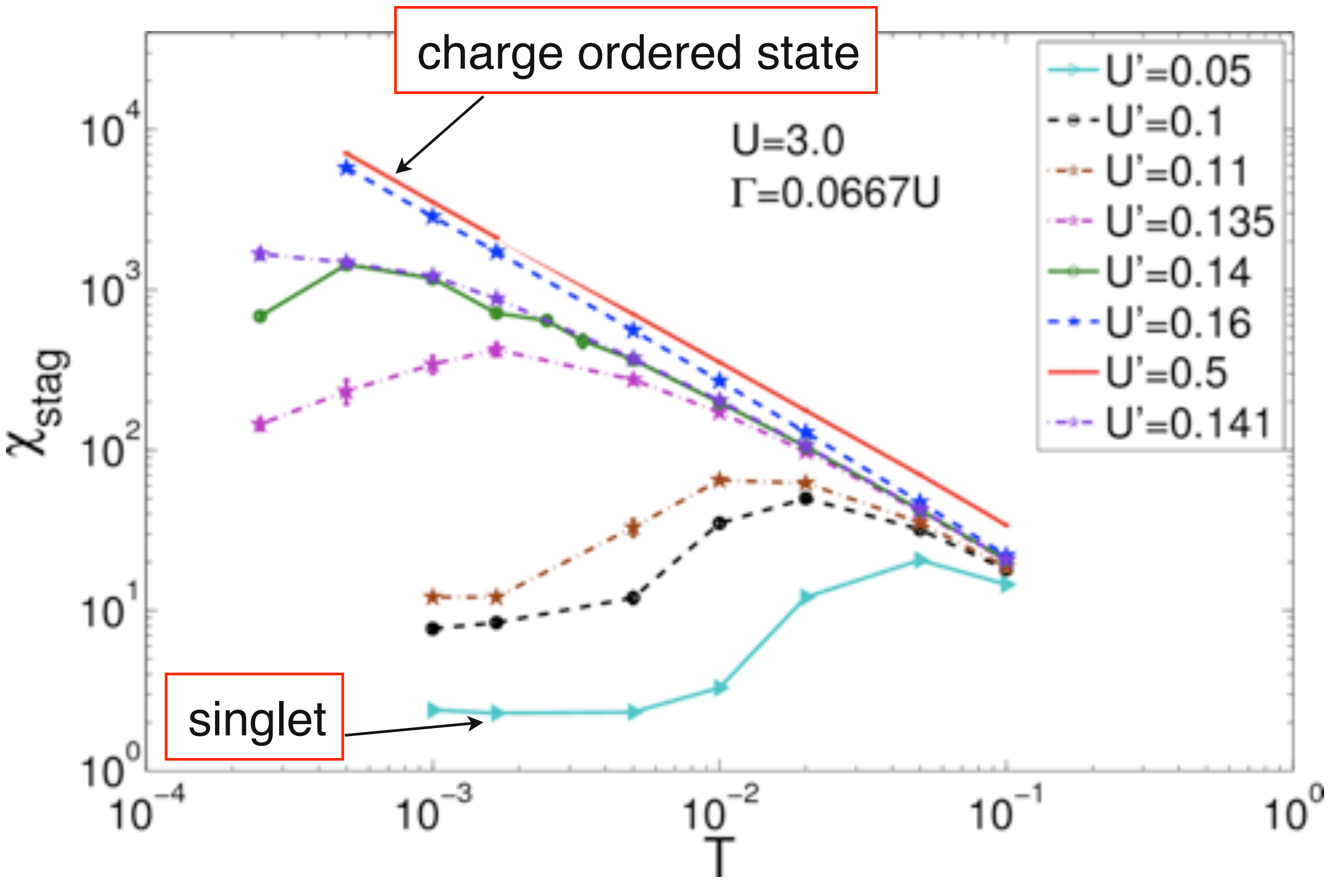
t/U≪1



Quantum Monte Carlo: Susceptibility

World line QMC with directed loop update (discretized imaginary time)

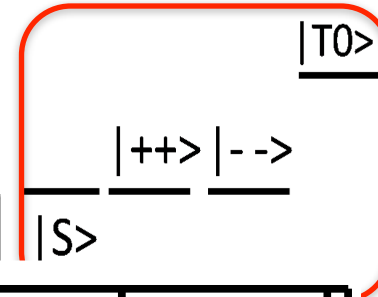
$$\hat{A} \equiv (n_{L+} + n_{R+}) - (n_{L-} + n_{R-}) \qquad \chi_{\text{loc}} \equiv \int_0^\beta d\tau \, \langle \hat{A}(\tau)\hat{A}(0) \rangle$$

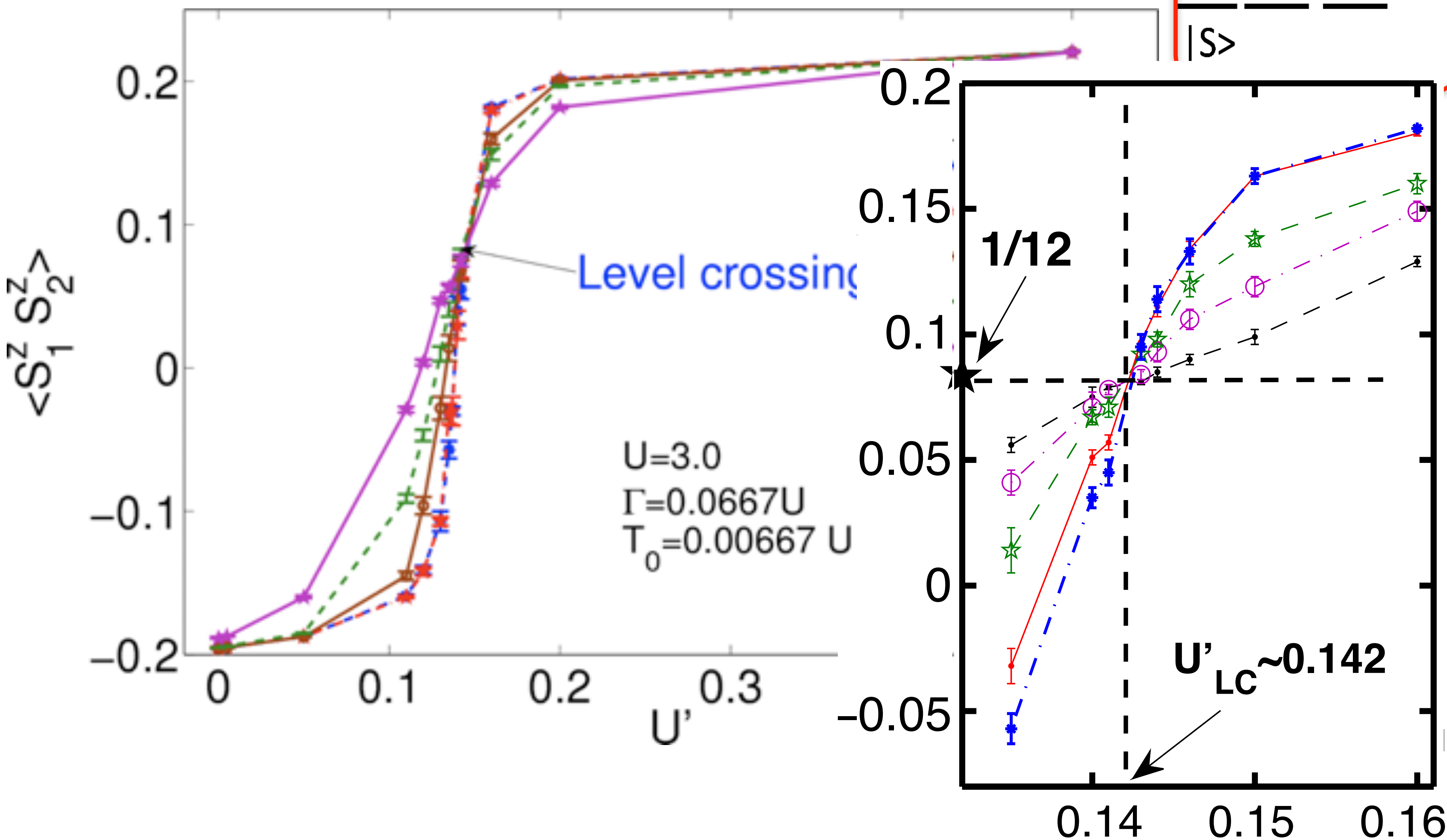


[Dong Liu]

Quantum Monte Carlo: Pseudospin Correlation

Calculate: $\langle\, S_L^z \, S_R^z \,\rangle$ $\qquad S_L^z \equiv \frac{1}{2}(n_{L+} - n_{L-})$





QMC: Conductance

Conductance can be evaluated by linear response formula:

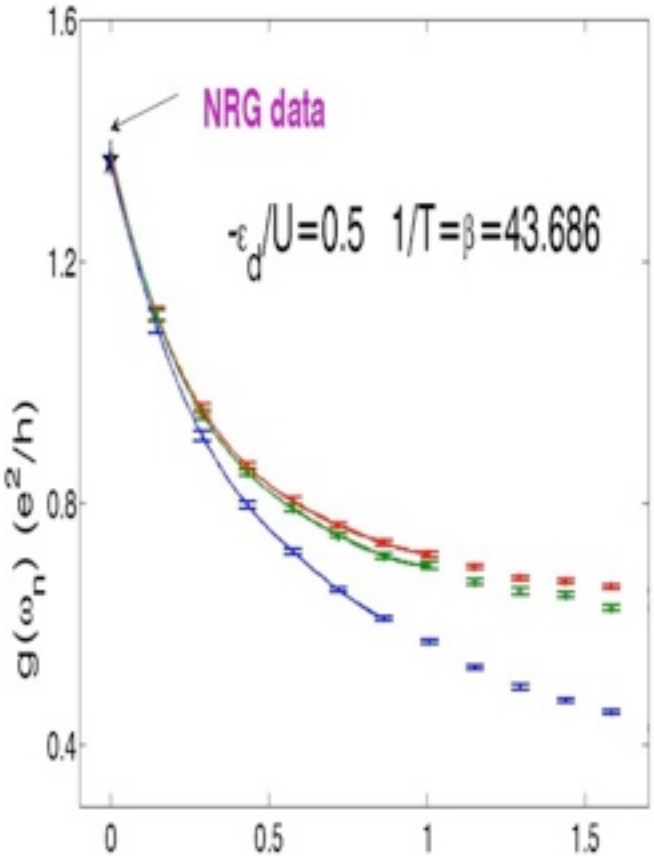
O. F. Syljuåsen, PRL (2007)

$$G = \lim_{\omega_n \to 0} g(i\omega_n)$$

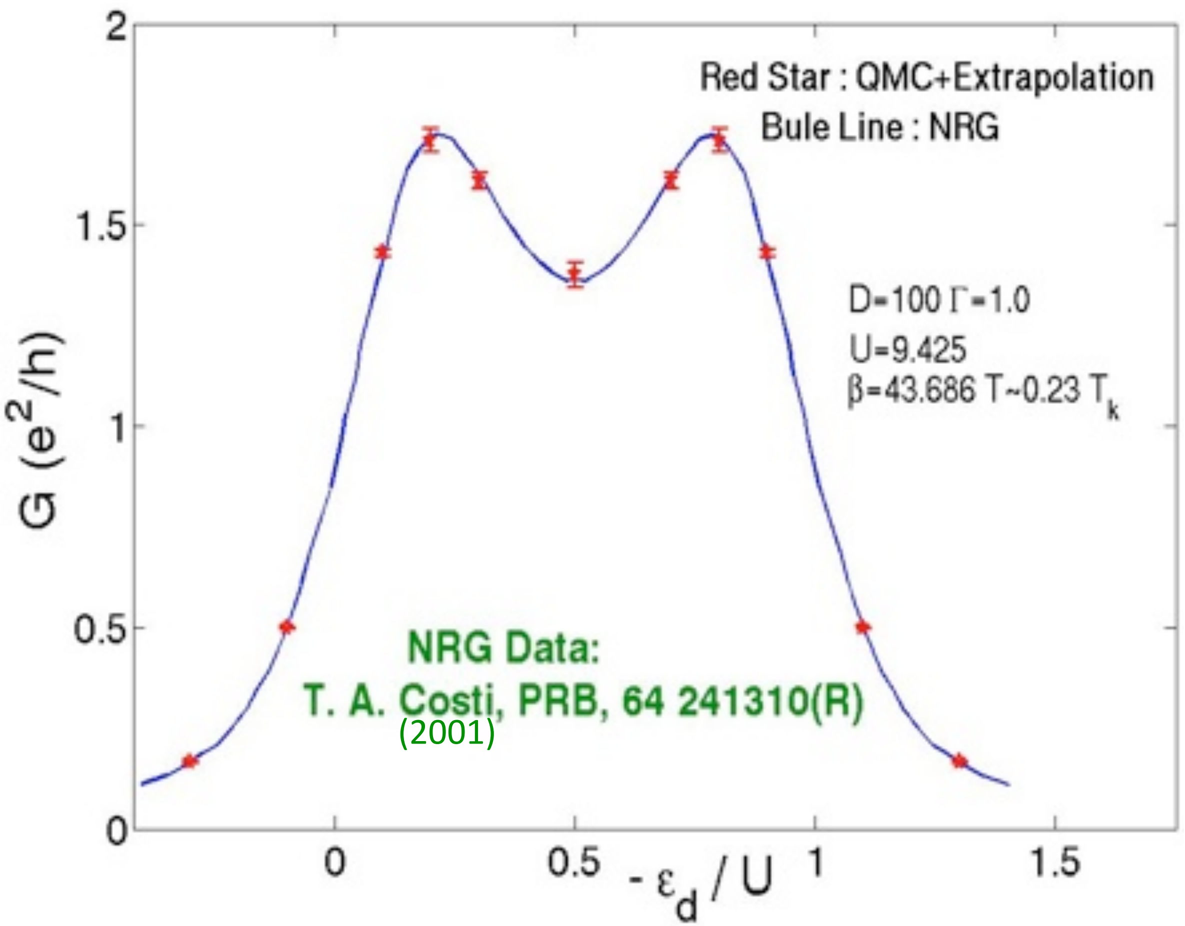
$$g(i\omega_n) \equiv \frac{\omega_n}{\hbar} \int_0^\beta d\tau \, \cos(\omega_n \tau) \, \langle P_x(\tau) P_y(0) \rangle$$

Matsubara frequency

$$P_x(\tau) \equiv \sum_{z>x} n_z(\tau)$$



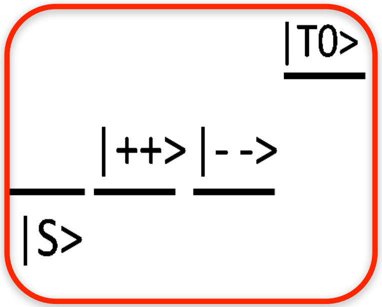
Matsubara Frequencies

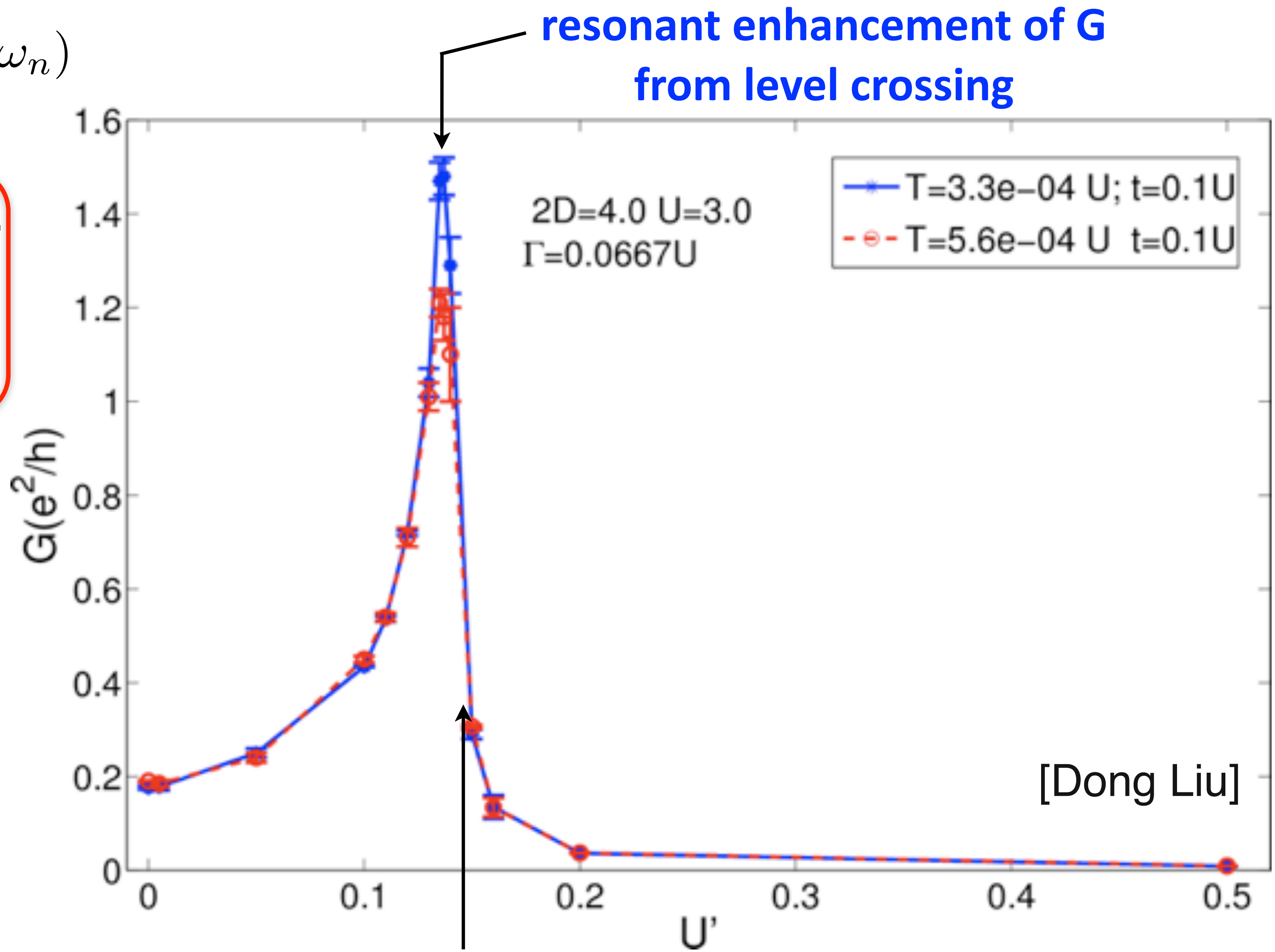


Conductance extrapolation works for regular Kondo

QMC: Conductance in Quadruple Dots

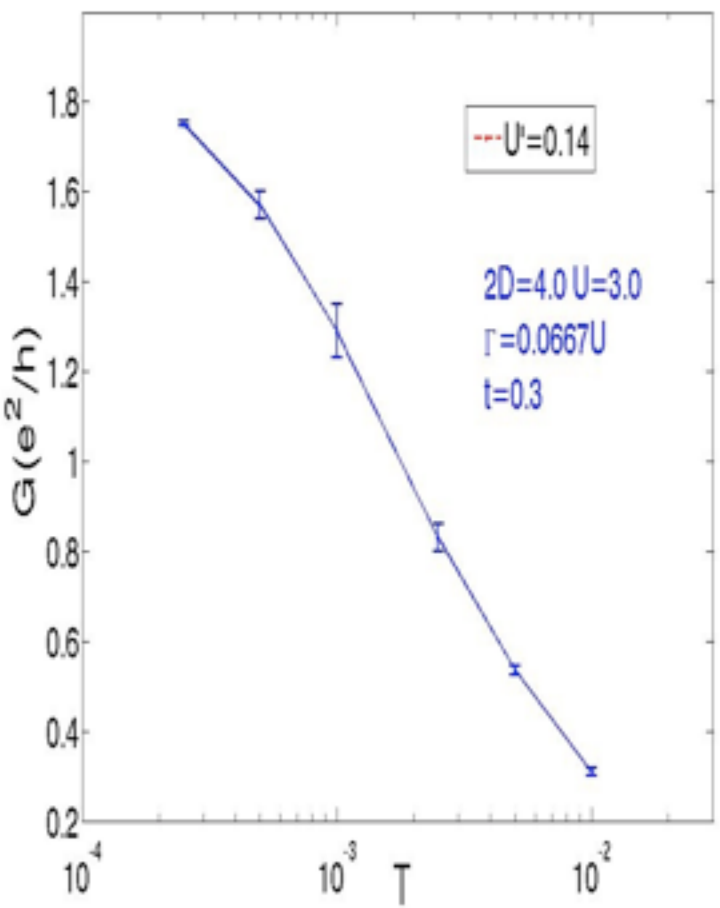
$$G = \lim_{\omega_n \to 0} g(i\omega_n)$$



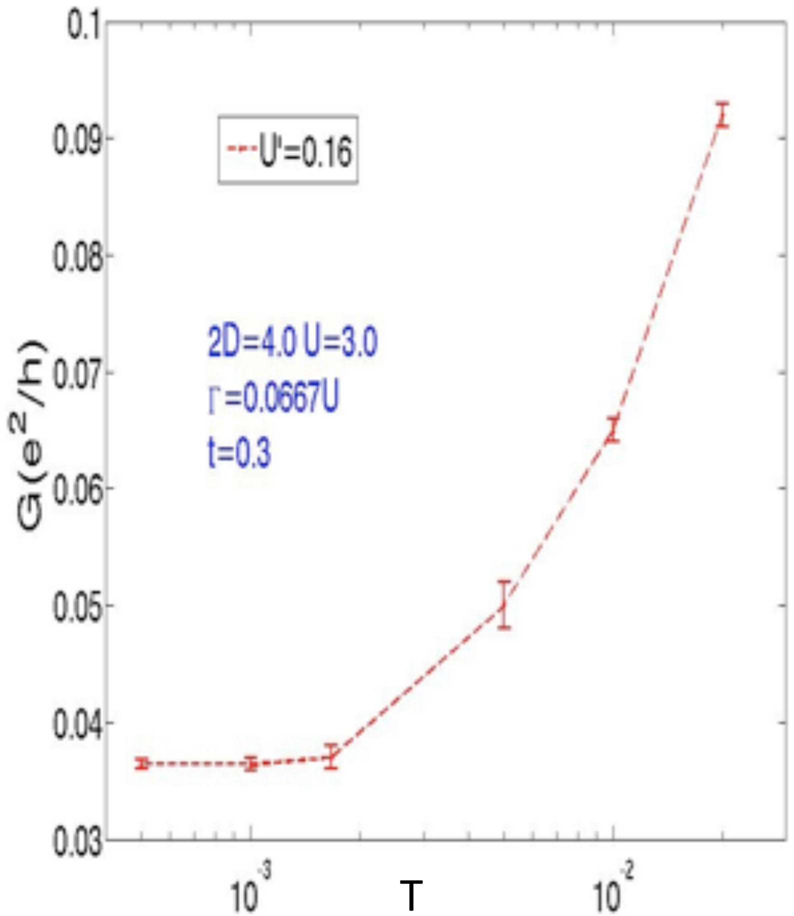


KT quantum phase transition; universal jump in conductance!

Temperature Dependence of G Near Transition

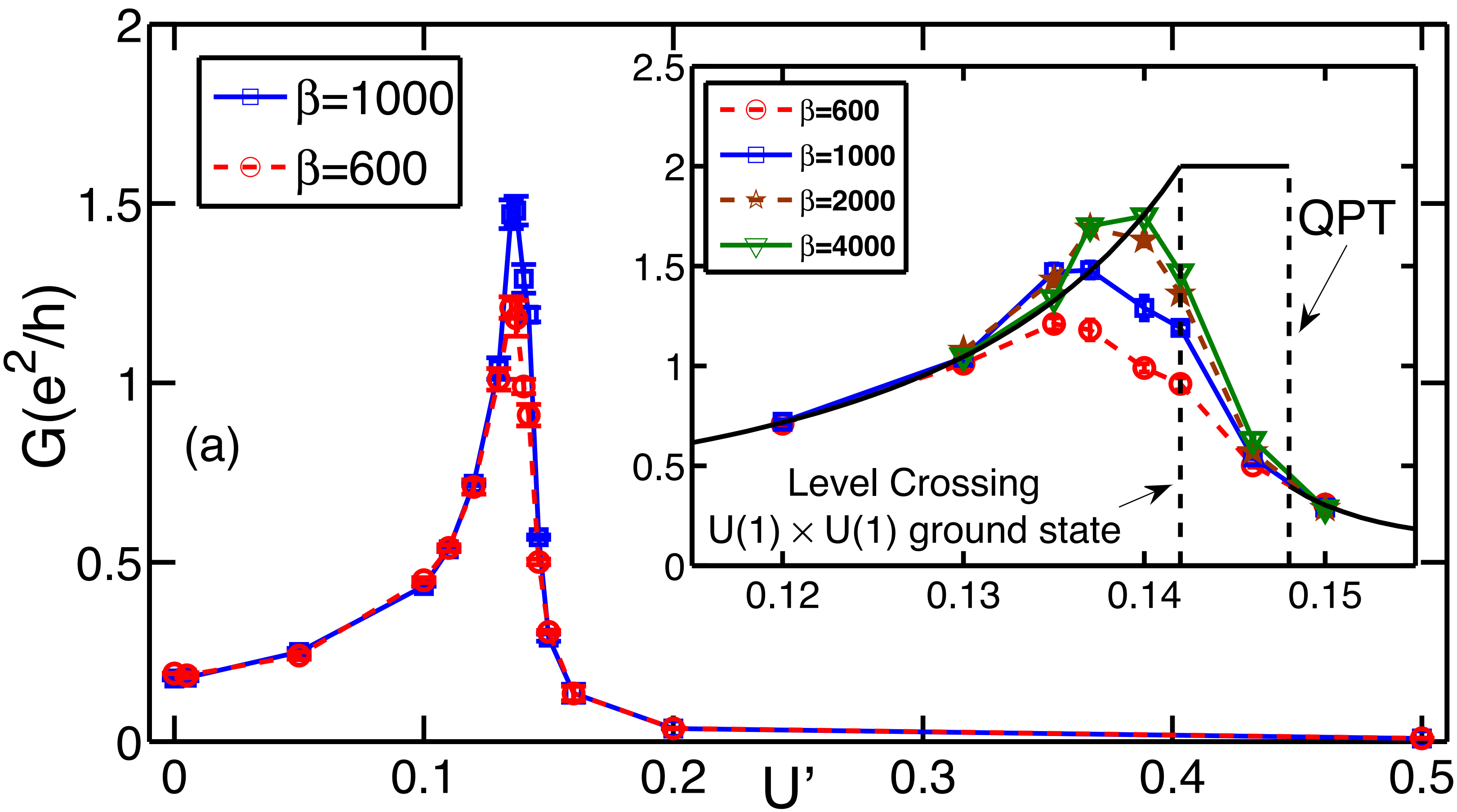


slightly below QPT



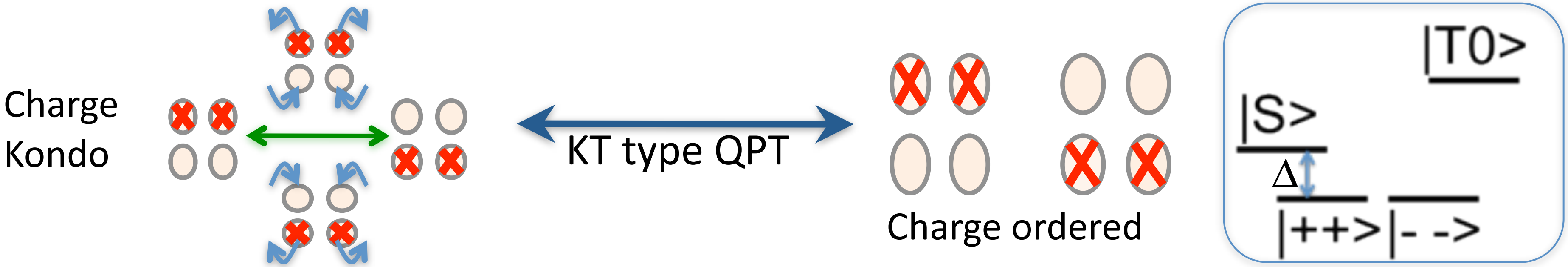
slightly into charge-ordered phase

Conductance Near the Level Crossing



[Dong Liu]

Low Energy Effective Theory Near QPT



Garst, et.al. PRB (2004); Galpin, et.al. PRL (2005) & J.Phys.Cond.Mat. (2006)

Schrieffer-Wolff transformation yields effective Hamiltonian:

$$H^{\rm eff}_{\rm CO} = \sum_{k,s=L/R,\sigma=+/-} \epsilon_{ks\sigma} c^+_{ks\sigma} c_{ks\sigma} + K \sum_{kk'\, s\sigma} \Big(\hat{n}_{L\sigma}+\hat{n}_{R\sigma}-1\Big) c^+_{ks\sigma} c_{k'\, s\sigma}$$

What about effect of spin flips?:

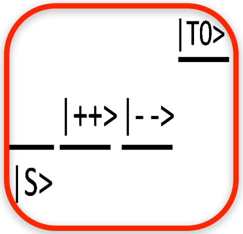
$$H^{\rm eff}_{\rm flip} = A \sum_{k,k',q,q'} \Big(|++\rangle\langle --|\, c^+_{kL-} c_{k'\, L+} c^+_{qR-} c_{q'\, R+} + \text{h.c.}\Big)$$

Naive scaling dimension of $H^{\rm eff}$ is <0 ➔ irrelevant operator

But, shift of electrons in the lead causes orthogonalty catastrophe, $H^{\rm eff}$ can become relevant for sufficiently small **Δ** ➔ no charge order.

Our work: check similarly that tunneling t doesn't change the story, only where transition occurs.

Low Energy Effective Theory Near Level Crossing (1)



Schrieffer-Wolff Transformation ➔ Effective Hamiltonian

$$H^{\text{eff}}_{\text{Kondo}} = J^{\text{I}}_{\perp}(M^{\text{I}}_{+}S^{\text{I}}_{-}+M^{\text{I}}_{-}S^{\text{I}}_{+})+2J^{\text{I}}_{z}M^{\text{I}}_{z}S^{\text{I}}_{z}+J^{\text{II}}_{\perp}(M^{\text{II}}_{+}S^{\text{II}}_{-}+M^{\text{II}}_{-}S^{\text{II}}_{+})+2J^{\text{II}}_{z}M^{\text{II}}_{z}S^{\text{II}}_{z}$$

$$\begin{aligned} M^{\text{I/II}}_{+} &= \sqrt{2}(|++\rangle\langle S| \mp |S\rangle\langle --|) = (M^{\text{I/II}}_{-})^{\dagger} \\ M^{\text{I}}_{z} &= |++\rangle\langle ++| - |--\rangle\langle --| \\ M^{\text{II}}_{z} &= |++\rangle\langle ++| + |--\rangle\langle --| - 2|S\rangle\langle S| \end{aligned}$$

$$\begin{aligned} S^{\text{I}}_{\pm} &= (c^{\dagger}_{0,L\pm}c_{0,L\mp} - c^{\dagger}_{0,R\pm}c_{0,R\mp}) \\ S^{\text{I}}_{z} &= \frac{1}{2}\sum_{i=L,R}(c^{\dagger}_{0,i+}c_{0,i+} - c^{\dagger}_{0,i-}c_{0,i-}) \\ S^{\text{II}}_{\pm} &= (\pm c^{\dagger}_{0,R\pm}c_{0,L\mp} \mp c^{\dagger}_{0,L\pm}c_{0,R\mp}) \\ S^{\text{II}}_{z} &= \frac{1}{2}\sum_{s=+,-}(c^{+}_{0,Ls}c_{0,Rs} + c^{+}_{0,Rs}c_{0,Ls}) \end{aligned}$$

What is this strange model??

- S=1 SU(2)? No: there are 6 operators above
- SU(3)? No: (1) 2 operators are missing in the impurity-- $|++\rangle\langle --|$ $|--\rangle\langle ++|$
  (2) 6 operators in the lead form SO(4)-- not big enough
- SU(2)xSU(2) [ie. SO(4)]? No: impurity operators don't obey SO(4) algebra

Low Energy Effective Theory Near Level Crossing (2)

Poor man's scaling:

$$\frac{dJ_\perp^{\mathrm{I}}}{d\ln D} = -2\rho(J_\perp^{\mathrm{I}} J_z^{\mathrm{I}} + 3J_\perp^{\mathrm{II}} J_z^{\mathrm{II}})$$

$$\frac{dJ_\perp^{\mathrm{II}}}{d\ln D} = -2\rho(J_\perp^{\mathrm{II}} J_z^{\mathrm{I}} + 3J_\perp^{\mathrm{I}} J_z^{\mathrm{II}})$$

$$\frac{dJ_z^{\mathrm{I}}}{d\ln D} = -2\rho[(J_\perp^{\mathrm{I}})^2 + (J_\perp^{\mathrm{II}})^2]$$

$$\frac{dJ_z^{\mathrm{II}}}{d\ln D} = -4\rho J_\perp^{\mathrm{I}} J_\perp^{\mathrm{II}}$$

Couplings diverge at some scale D_0 which can be taken as Kondo temp.

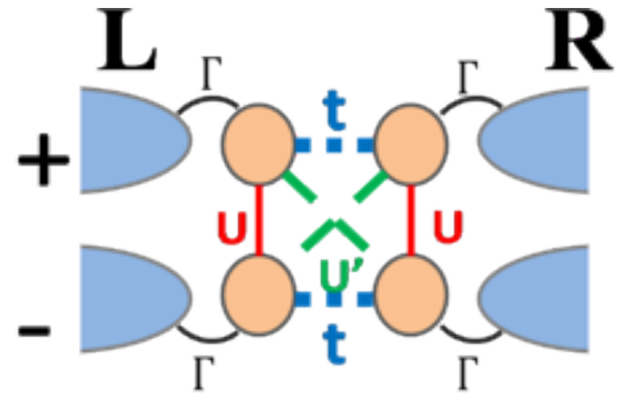
$$\lim_{D\to D_0} J_\perp^{\mathrm{I}} : J_\perp^{\mathrm{II}} : J_z^{\mathrm{I}} : J_z^{\mathrm{II}}$$

$$\to \sqrt{2} : \sqrt{2} : 1 : 1$$

more symmetry at the strong coupling fixed point (dynamically enhanced)

Low Energy Effective Theory Near Level Crossing (3)

What is the symmetry??



Symmetry of effective Hamiltonian:

$$U(1)_{\text{charge}} \times U(1)_{\text{pseudospin}} \times Z_{2,\pm} \times Z_{2,\text{left-right}}$$

For instance, $U(1)_{\text{pseudospin}}$ is generated by $S^{\mathrm{I}}_{z,\text{Tot}} \equiv M^{\mathrm{I}}_z + \sum_k S^{\mathrm{I}}_{z,k}$

Well, what about $S^{\mathrm{II}}_{z,\text{Tot}} \equiv M^{\mathrm{II}}_z + \sum_k S^{\mathrm{II}}_{z,k}$

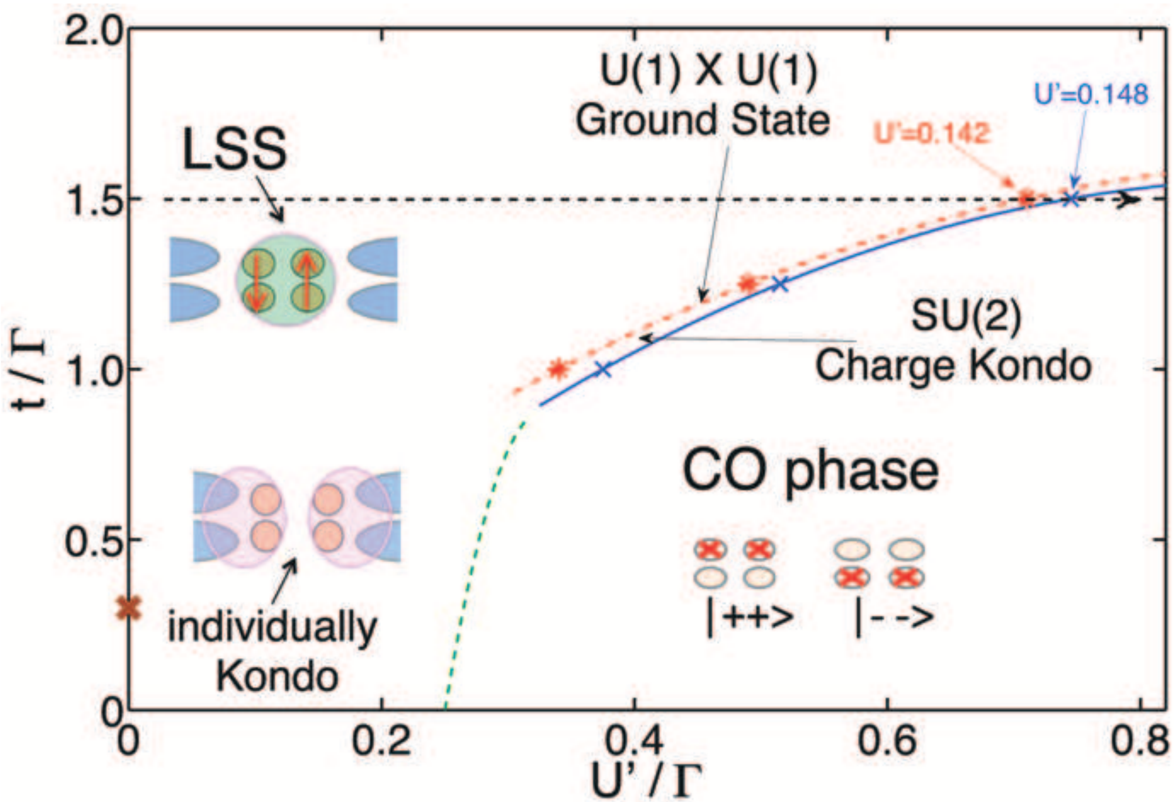
does **not** commute with bare H, but **does** commute with the strong coupling Hamiltonian

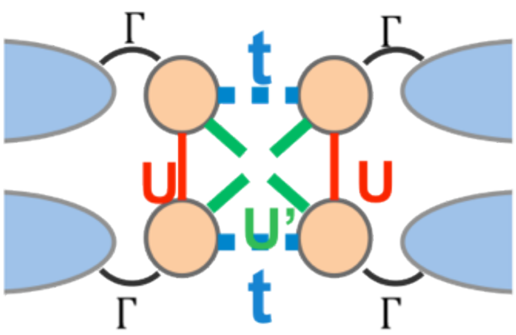
a π rotation of this type generates $Z_{2,\text{left-right}}$

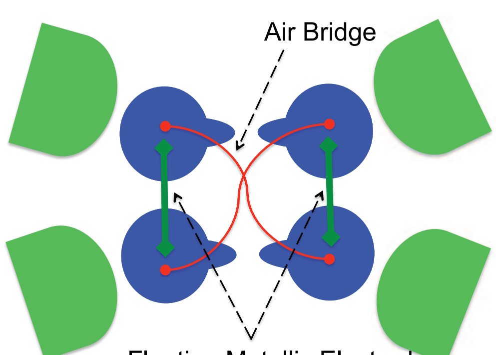
$$\boxed{Z_{2,\text{left-right}} \longrightarrow U(1)_{\text{left-right}}}$$

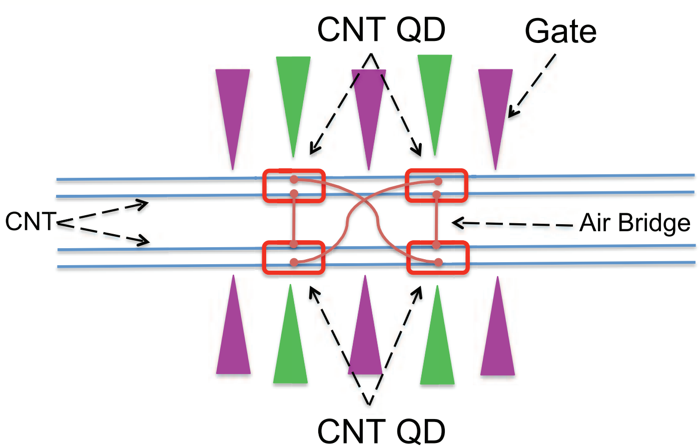
➔ conductance

Phase Diagram



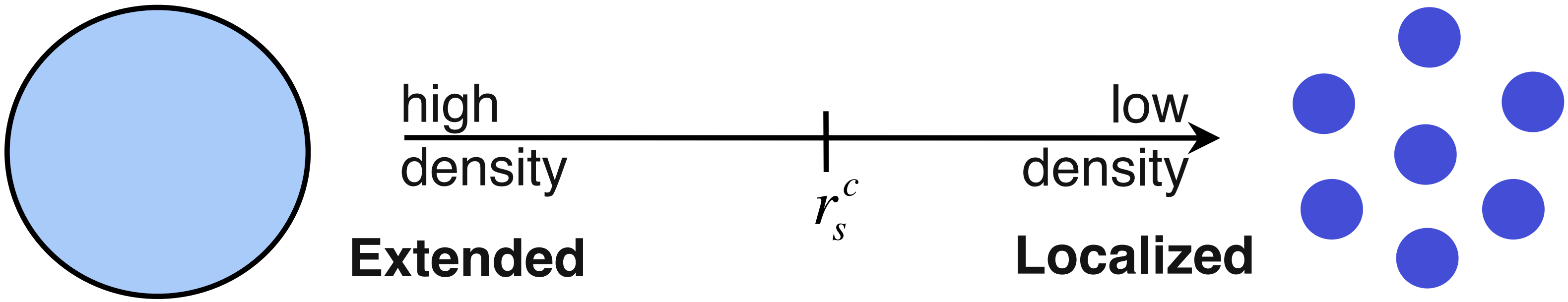






Interaction-Induced Localization in an Inhomogeneous Quantum Wire

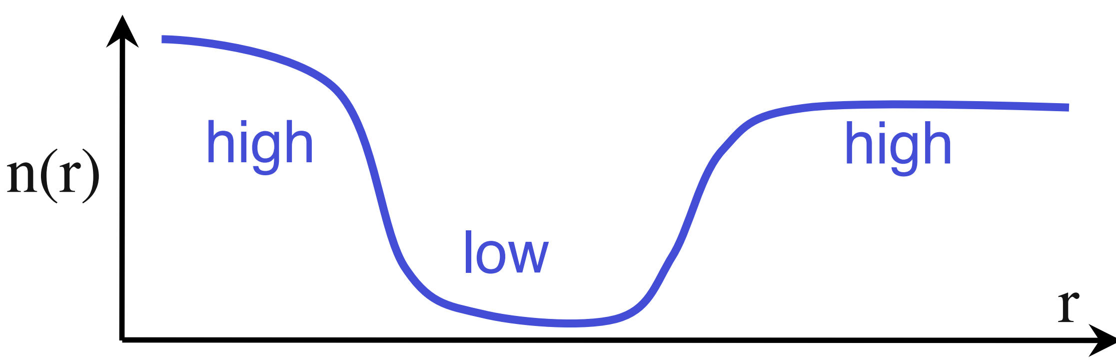
(Devrim Güçlü, Amit Ghosal, Hong Jiang, Cyrus Umrigar, and HUB)



Parametrize interaction strength:
ratio of interaction strength to kinetic energy

$$r_s^{2D} \equiv \frac{1}{\sqrt{\pi n a_0}} \qquad r_s^{1D} \equiv \frac{1}{2 n a_0}$$

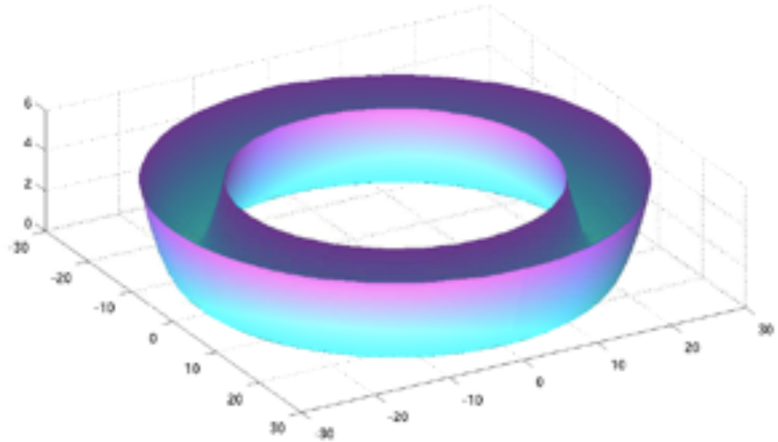
How will such physics appear in an inhomogeneous system?



- interface between liquid & crystal ?
- broken translational invariance → smaller r_s^c ?

Model: Quasi-1D Wire with Depleted Region

$$\boxed{H = -\frac{1}{2}\sum_{i}^{N}\nabla_i^2 + \sum_{i}^{N}V(\mathbf{r}_i) + \sum_{i<j}^{N}\frac{1}{r_{ij}}}$$



$$V(\mathbf{r}) = \frac{1}{2}\omega^2(\mathbf{r}-\mathbf{r}_0)^2 + V_{sg}(\tanh(s(\theta+\theta_0)) - \tanh(s(\theta-\theta_0)))$$

- 2D electrons confined to a ring – Coulomb interaction
- transverse confinement is harmonic
- V_{sg} depletes electrons in a certain region
- parameter “s” controls steepness of the potential
- narrow ring – only one transverse channel

Typically: N ~ 30; size of depleted region ~0.3-0.7 μm for GaAs

Tool: Variational and Diffusion Quantum Monte Carlo

VMC followed by DMC with fixed node approximation

based on variational principle: $E_{VMC} = \frac{\int \Psi_T^*(\mathbf{R})\mathcal{H}\Psi_T(\mathbf{R})d\mathbf{R}}{\int \Psi_T^*(\mathbf{R})\Psi_T(\mathbf{R})d\mathbf{R}} \geq E_{GS}$

trial wave-function:

$$\Psi_T = J\left\{\sum_n d_n D_n^{\uparrow} D_n^{\downarrow}\right\}$$

Jastrow part, $J = \prod_{i<j} exp\left\{ar_{ij}/(1+br_{ij})\right\}$
$\Rightarrow$ induces correlations.
(actual Jastrow used much more complex)

- Slater dets taken with single particle (i) DFT orbitals or (ii) Gaussians
  - agree to high accuracy – can use either one

  includes near-degeneracy and dynamic correlation
- use DMC on optimized wavefunction to project out the ground state

  apply $\exp\{-\tau H\}$
- used previously for circular quantum dots:

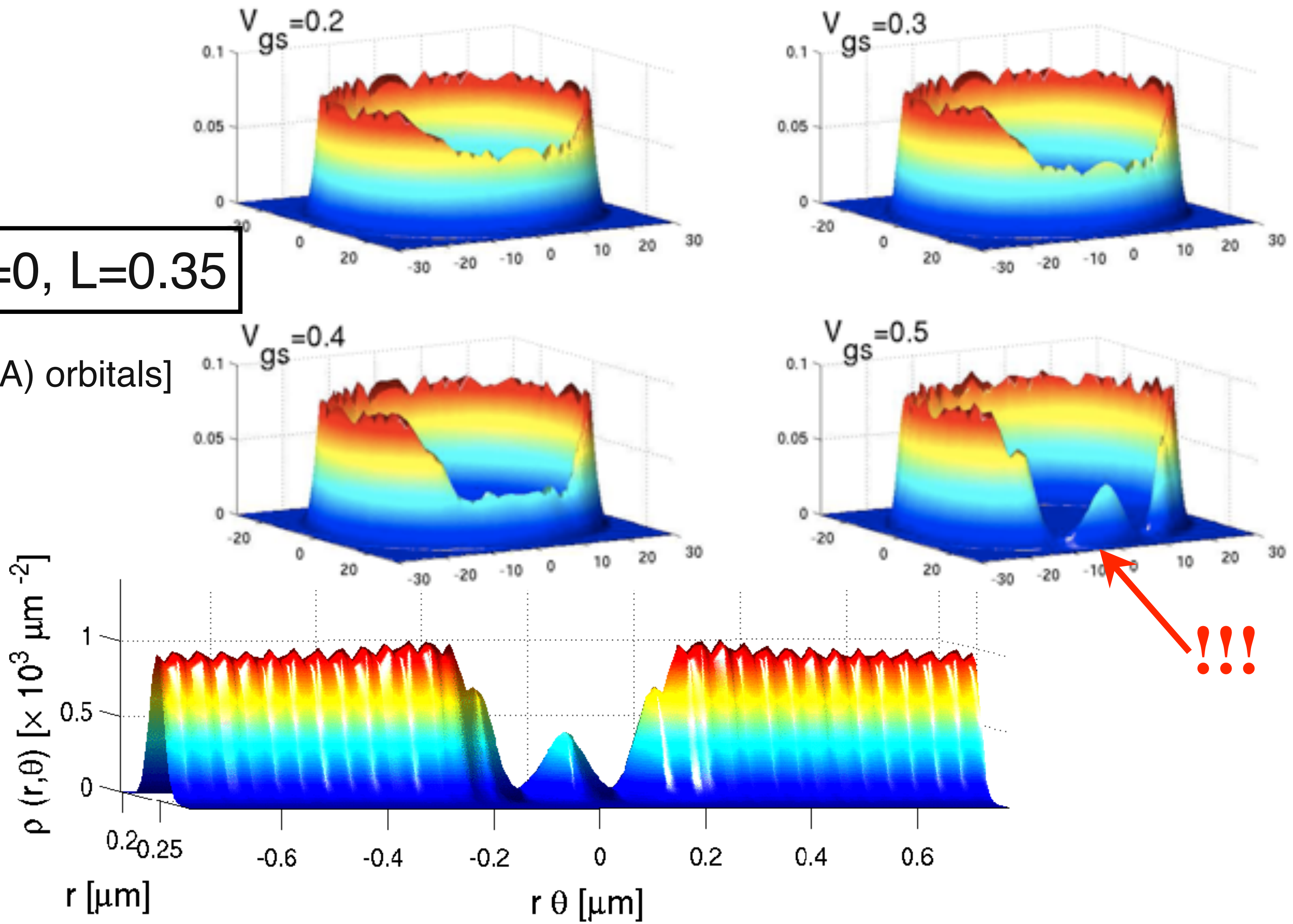
  compared with exact diagonalization for N=3, 4 and 6

[Cyrus Umrigar]

Density: Depleting a Short Constriction

N=30, S=0, L=0.35

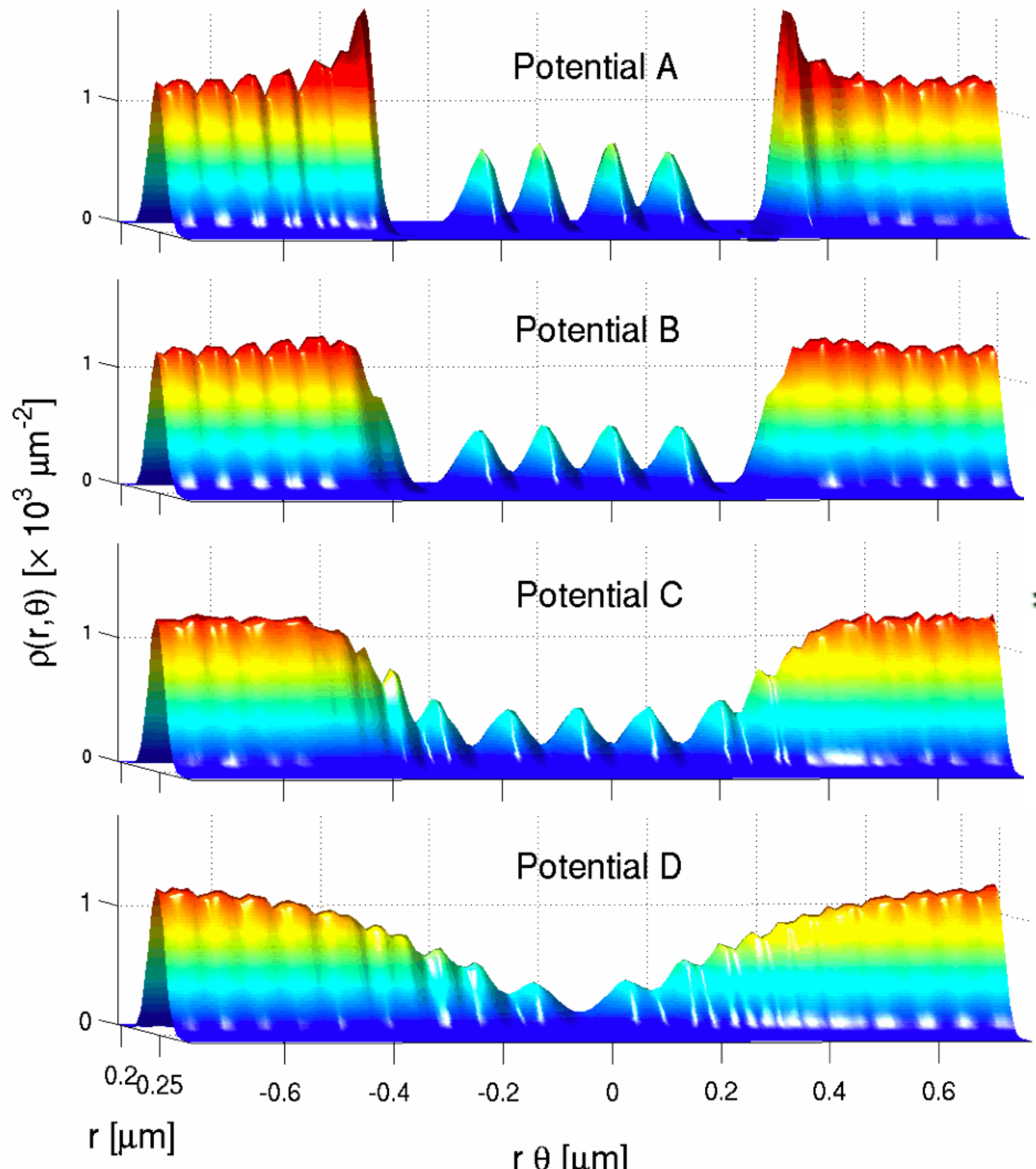
[liquid (LSDA) orbitals]



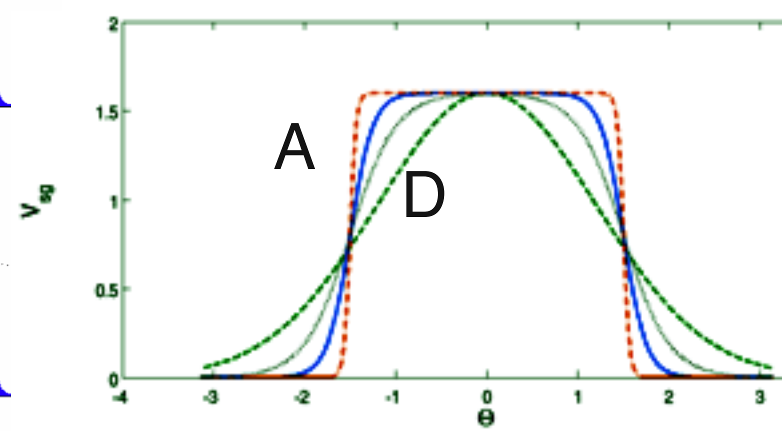
[Devrim Güçlü]

Density: Long Constriction, Steepness of Potential

N=31, L=0.7



steep external potential



smooth external potential

[Devrim Güçlü]

[floating Gaussian orbitals]

CONCLUSIONS

Tunable Strong Correlations in Quantum Wires and Dots

➡ **QPT and Kondo resonance in quadruple quantum dots**

- may provide experimental access to a **charge-ordered QPT:** KT type, universal jump in the conductance
- **resonance:** triple level degeneracy ➔ conductance peak "Kondo" associated with peculiar symmetry enhancement

Dong Liu, S. Chandrasekharan, HUB

➡ **Interaction-induced localization in a quantum wire**

- **nature of interface** controlled by steepness of external potential
- **sharp V_{ext}:** electrons trapped by dynamic barrier ➔ Coulomb blockade; do Kondo correlations form?
- **smooth V_{ext}:** in long constriction, smooth connection from liquid to crystal

Devrim Güçlü, Amit Ghosal,
Hong Jiang, Cyrus Umrigar, HUB