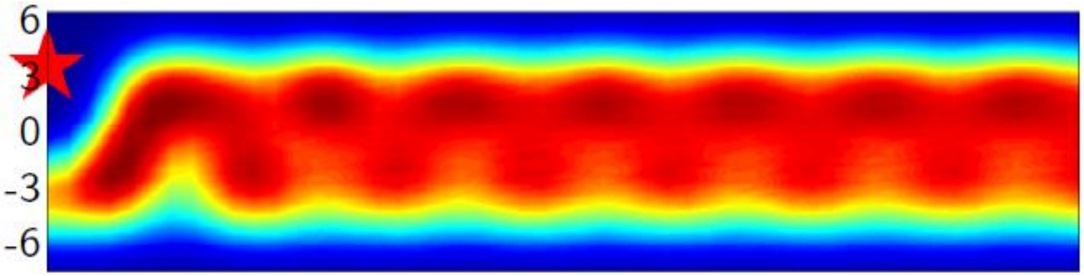
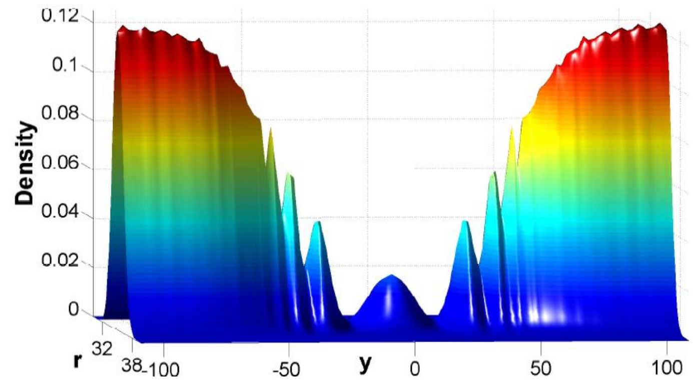
Zigzag Phase Transition in Quantum Wires and Localization in Constrictions





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Phys. Rev. Lett. **110,** 246802 (2013)

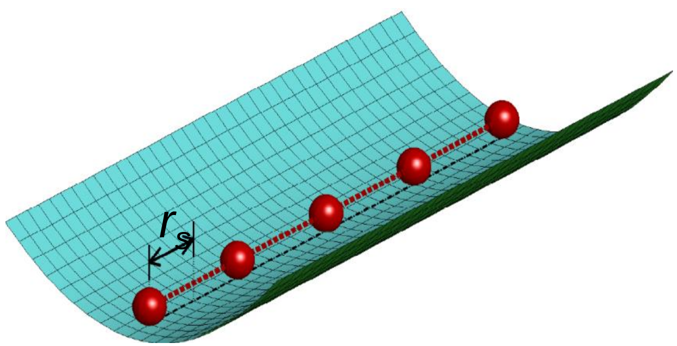
Supported by the Department of Energy

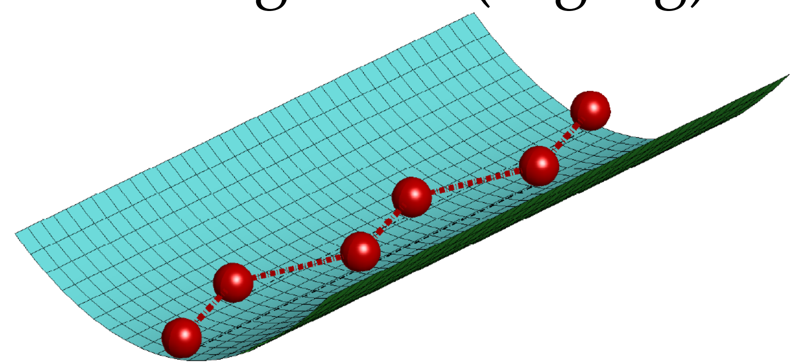
Outline: The Interacting 1D Electron Gas

Reduced dimensionality enhances correlations

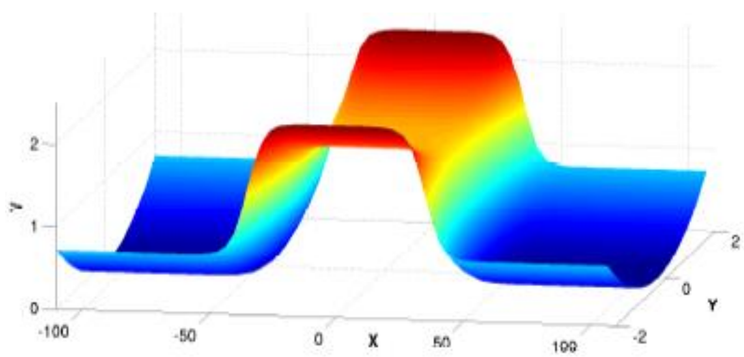
- Homogeneous 1D systems well understood theoretically
- 1D physics is fundamentally different from higher-dimensional physics; the real world is 3D!

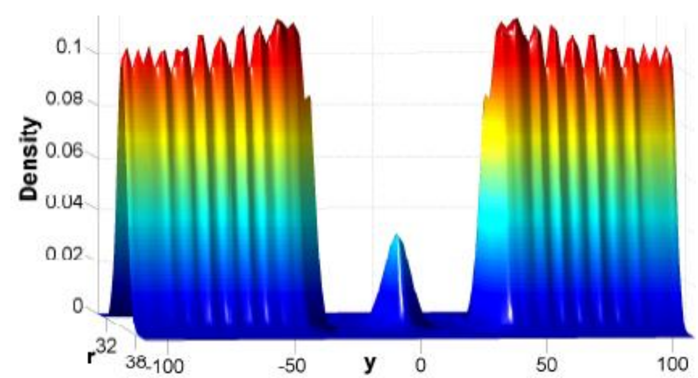
  → We study the transition from 1D to higher-D (Zigzag)





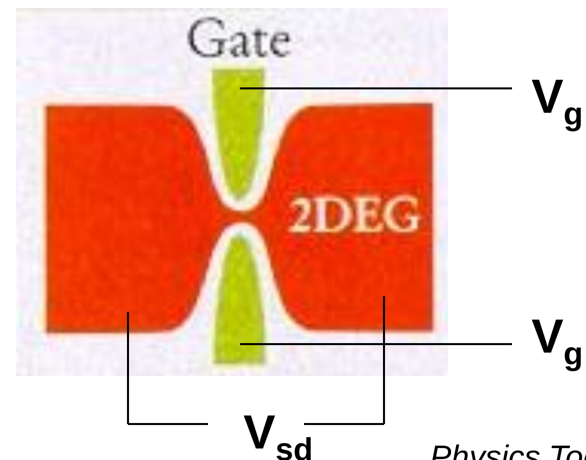
- We study the role of inhomogeneity (QPC)



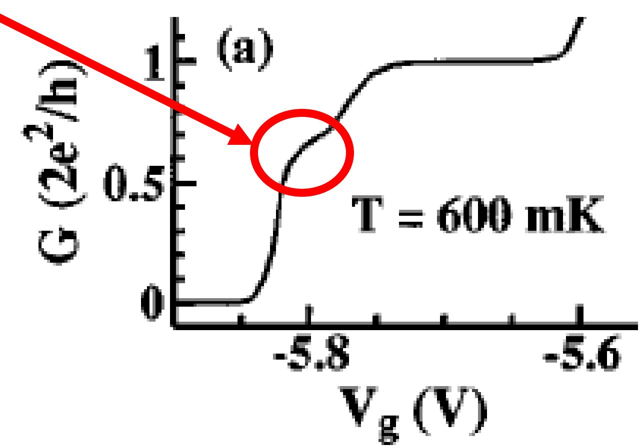


1D electron systems

- Carbon nanotubes, certain organic salts, electrons floating on liquid He, cleaved edge overgrowth quantum wires, Linear ion traps, …
- Quantum Point Contacts (QPC's)
  - 2DEG reservoirs separated by narrow 1D constriction
  - Variety of interesting, unexplained experimental effects
  - Expect conductance through QPC quantized in units of $2e^2/h$; Extra unexpected structure at 0.7 $(2e^2/h)$! ("0.7 Anomaly")
  - Bound states
  - Possible row coupling



Physics Today

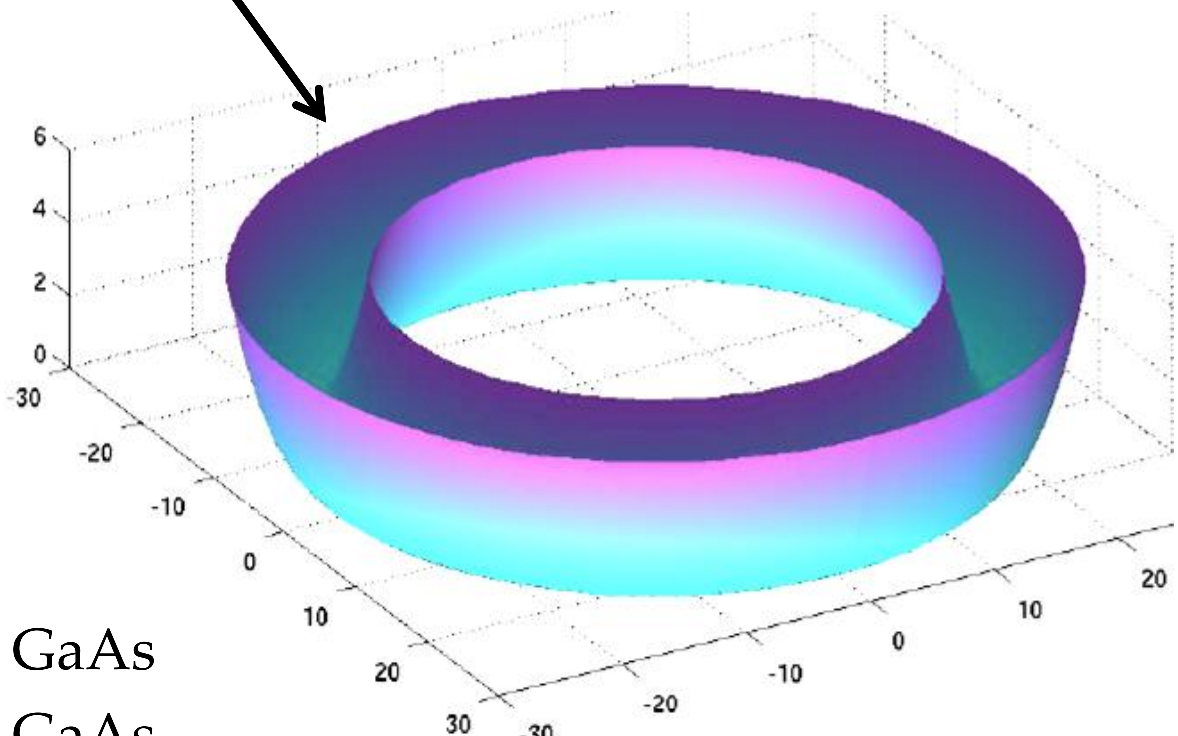


Thomas et al. PRL **77** 135 (1996)

Model: Quantum Ring (Wire)

- N electrons confined to ring (quasi-1D system)

$$H = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 + \frac{1}{2}\sum_{i=1}^{N}\omega^2(r_i - r_{Ring})^2 + \sum_{i<j\le N}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$



- $\omega = 0.1, 0.6$
- $r_s = 0.5 - 5.0$
- Experimentally relevant to GaAs QPC's
  (Rossler et al., Hew et al.)

Use atomic units:

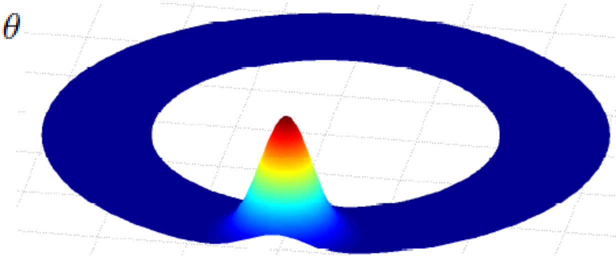
$a_0^* \equiv \hbar^2\varepsilon/m^*e^2 = 9.8$ nm in GaAs

$H^* \equiv e^2/\varepsilon a_0^* = 11.9$meV in GaAs

Method: Variational and Diffusion Monte Carlo

- Variational Monte Carlo (VMC):
  - Trial wavefunction: $\psi_t(R) = J(R) D^{\uparrow} D^{\downarrow}$

  D↑,D↓ - Slater Determinants of single particle orbitals
    - Planewaves $\psi_{\text{planewave}}(r,\theta) = \phi_{n,k_\theta}(r) e^{\pm i k_\theta \theta}$
    - LSDA
    - Floating Gaussians



$$\psi_{r_c,\theta_c,\omega_r,\omega_\theta}(r,\theta) \propto \sqrt{\omega_r} \exp\left(\frac{-\omega\omega_r (r-r_c)^2}{2}\right) \exp\left(\frac{\omega_\theta[\cos(\theta-\theta_c)-1]}{2}\right)$$

  - ***J(R)*** – Jastrow Factor – incorporates correlations
- Diffusion Monte Carlo (DMC)
  - Project out ground state:

$$|\psi(\tau)\rangle = e^{-(\hat{H}-E_t)\tau} |\psi(0)\rangle, \text{ apply repeatedly}$$

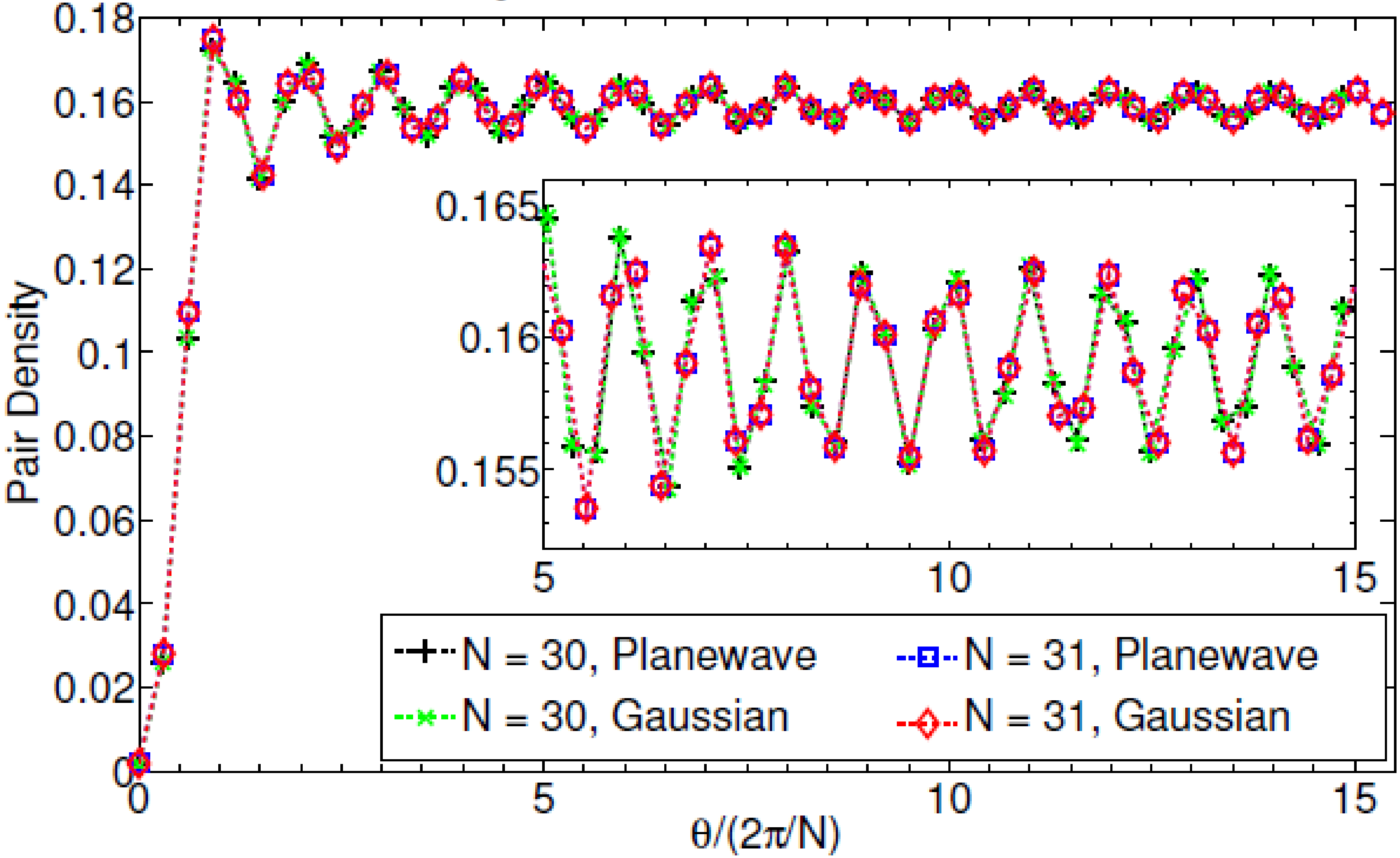
Fixed Node Approximation (Fermion sign problem)

Comparison of VMC Single Particle Orbitals

- Similar QMC pair densities starting from different orbitals

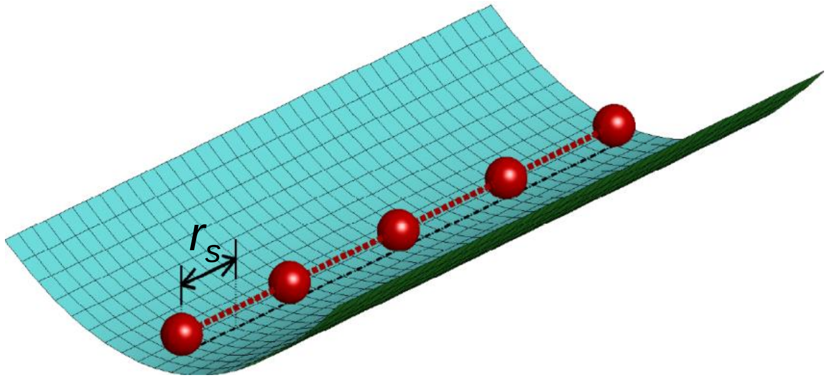
$$\langle \hat{\rho}(0)\hat{\rho}(\theta)\rangle \equiv \int \langle \hat{\rho}(r,\theta)\hat{\rho}(r_\star,0)\rangle \, r\,\mathrm{d}r\, r_\star\,\mathrm{d}r_\star$$

ω = 0.1
r_s = 4.0

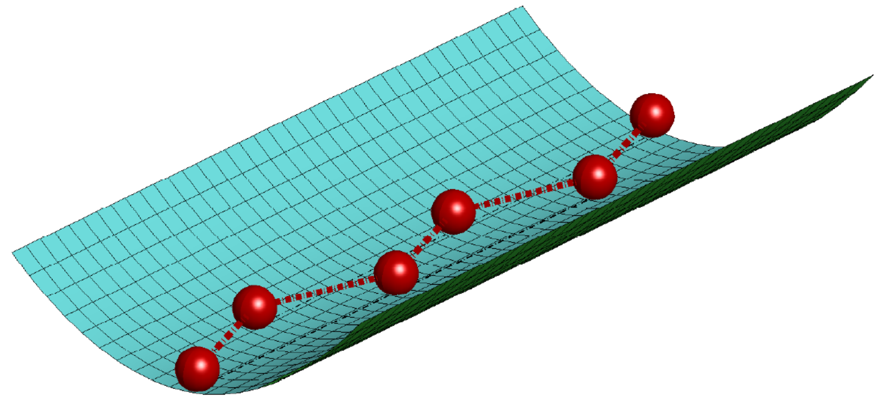


The Zigzag Transition

PRL **110**, 246802 (2013)



linear Wigner crystal



quasi-1D zigzag crystal

- Two length scales: $r_s = 1/(2na_B)$ and r_0,
  - r_0: Length where confinement $(1/2)m\omega^2 r_0^2$ is equal to Coulomb repulsion $e^2/\varepsilon r_0$

$$r_0 = \sqrt[3]{\frac{2e^2}{\varepsilon m\omega^2}}$$

- If r_s and r_0 are of same order, symmetry about axis of wire breaks → Transition to quasi-1D zigzag crystal
- Smaller ω (wider wire) → effectively stronger interaction.

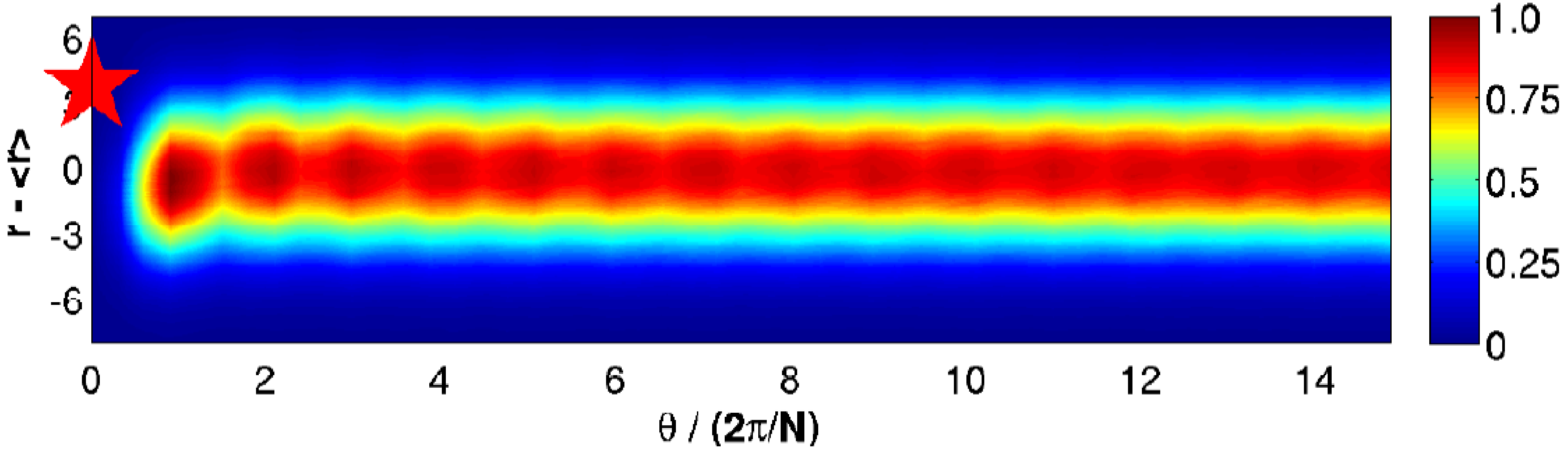
$\underline{\omega = 0.1}$, $r_0 = 5.85$:
$r_0 > 1$ means zigzag transition in localized Wigner Crystal regime.
Classical $r_s^{critical} = 3.75$

$\underline{\omega = 0.6}$, $r_0 = 1.77$:
more quantum case
Classical $r_s^{critical} = 1.14$

- Higher densities: zigzag order decreases, "liquid" (2 gapless modes)

Pair Density: Linear Wigner Crystal Regime

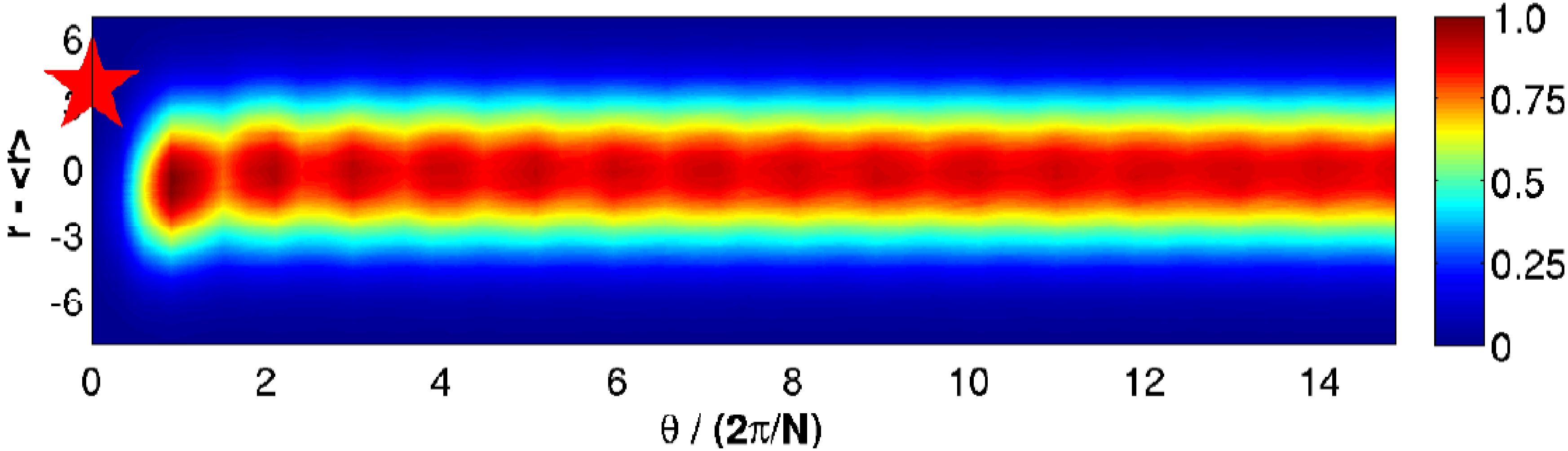
r_s **= 4.0,** $\omega = 0.1$: N localized peaks along axis of wire



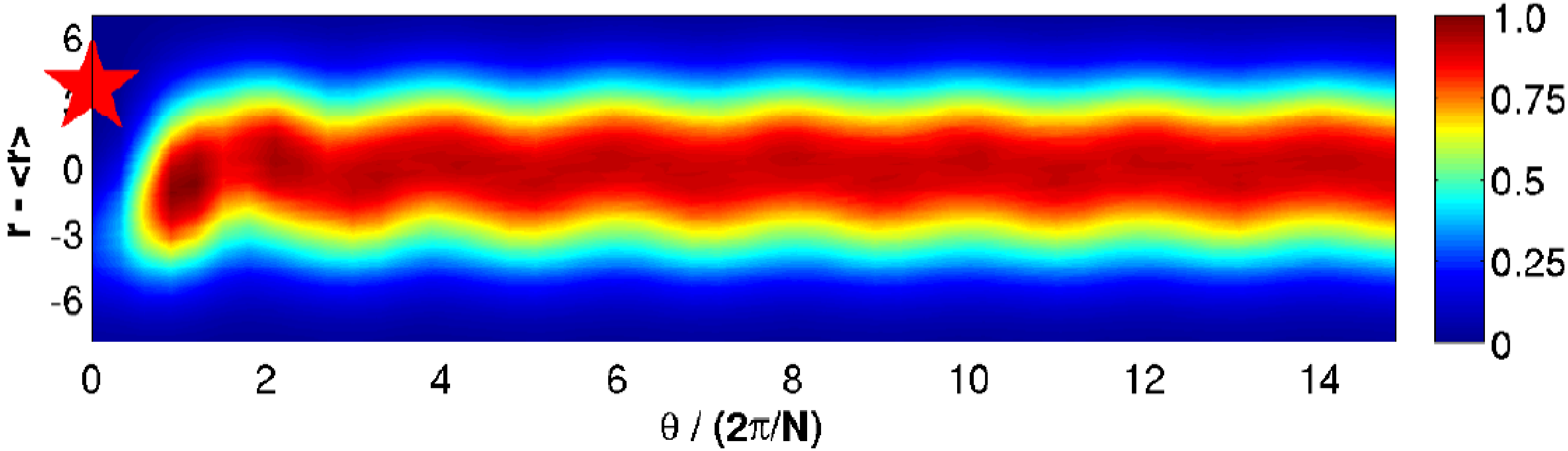
$$\langle \hat{\rho}(r,\theta)\hat{\rho}(r_\star,0)\rangle \,/\, \langle \hat{\rho}(r_\star,0)\rangle$$

Pair Density: Zigzag Regime (ω = 0.1)

r_s = **4.0**: N localized peaks along axis of wire

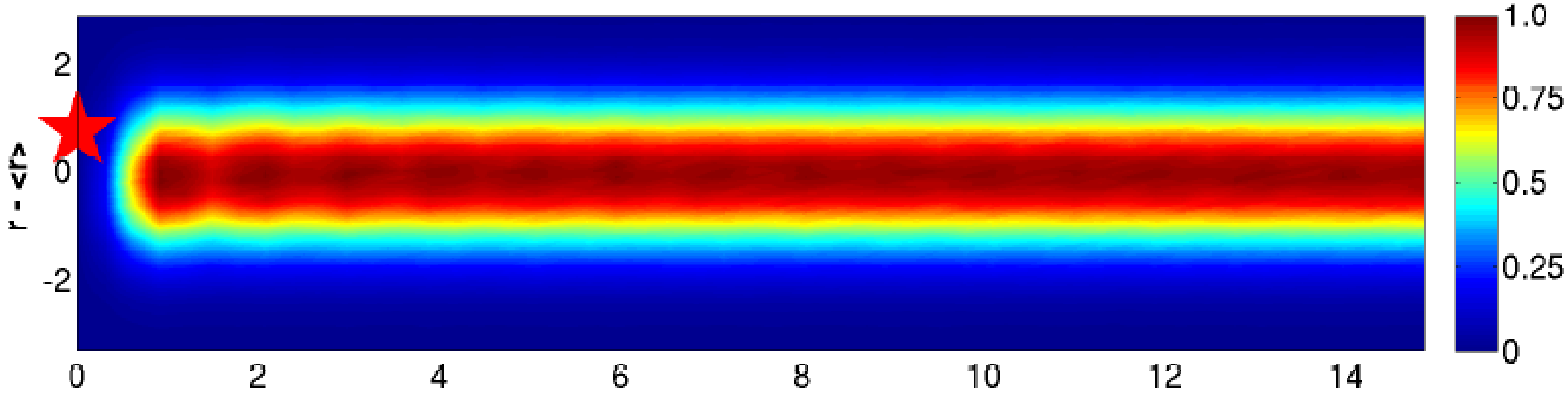


r_s = **3.6**: Zigzag structure



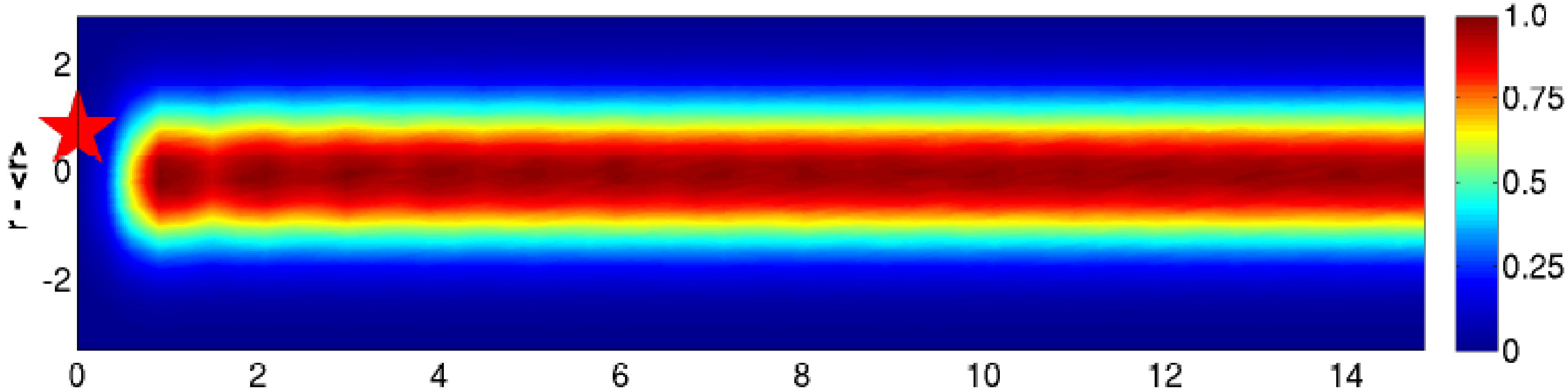
Pair Density: ω = 0.6

r_s **= 1.5**: Linear regime, weaker localization

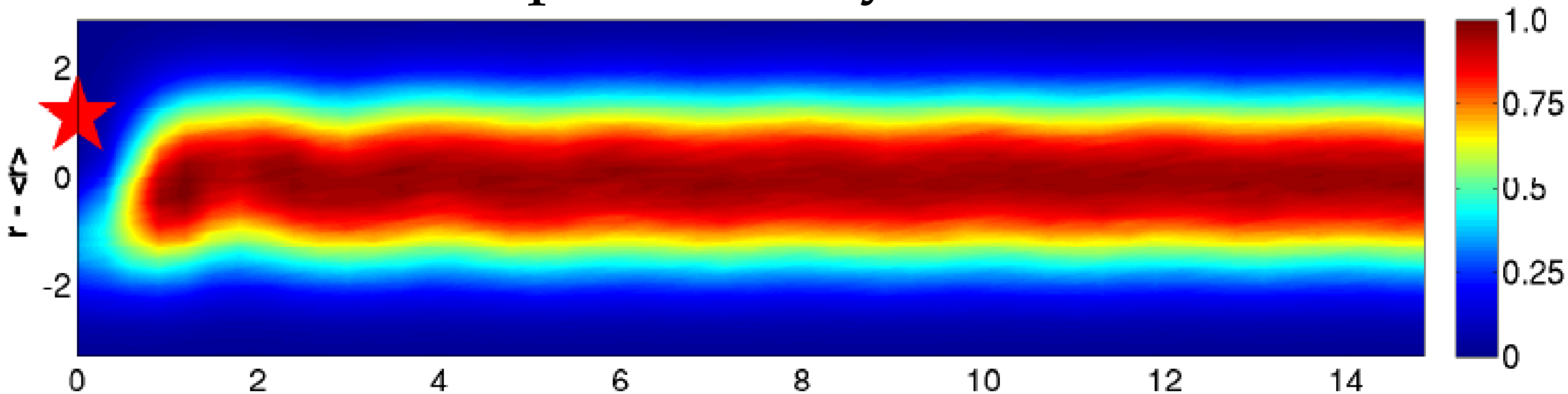


Pair Density: ω = 0.6

r_s = **1.5**: Linear regime, weaker localization

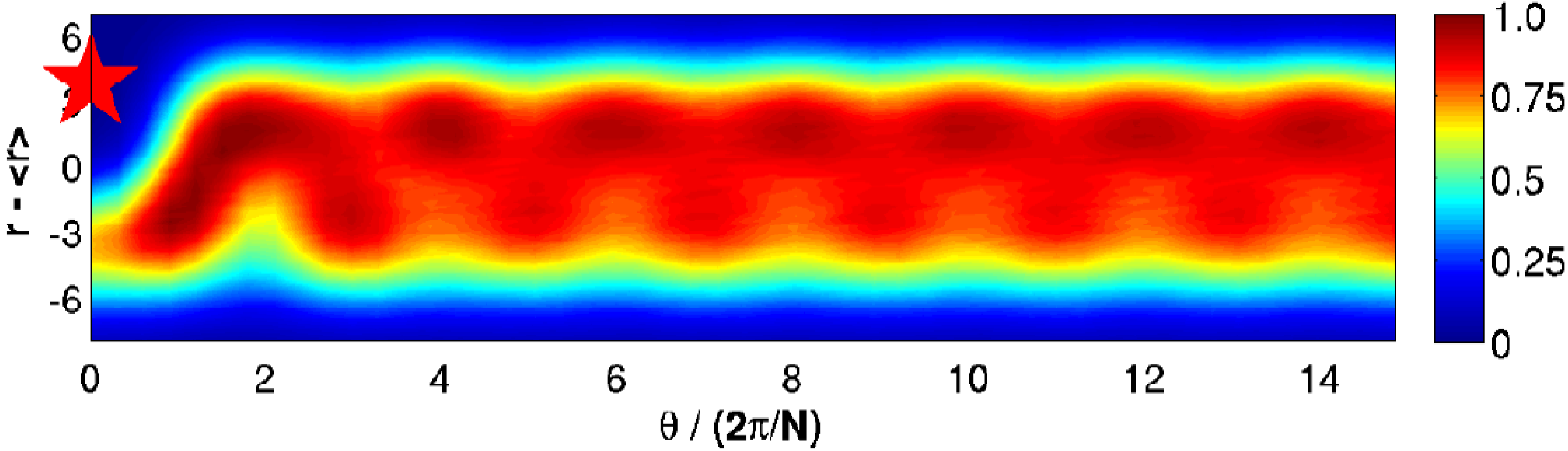


r_s = **1.3**: Zigzag regime, but quantum fluctuations blur features in pair density

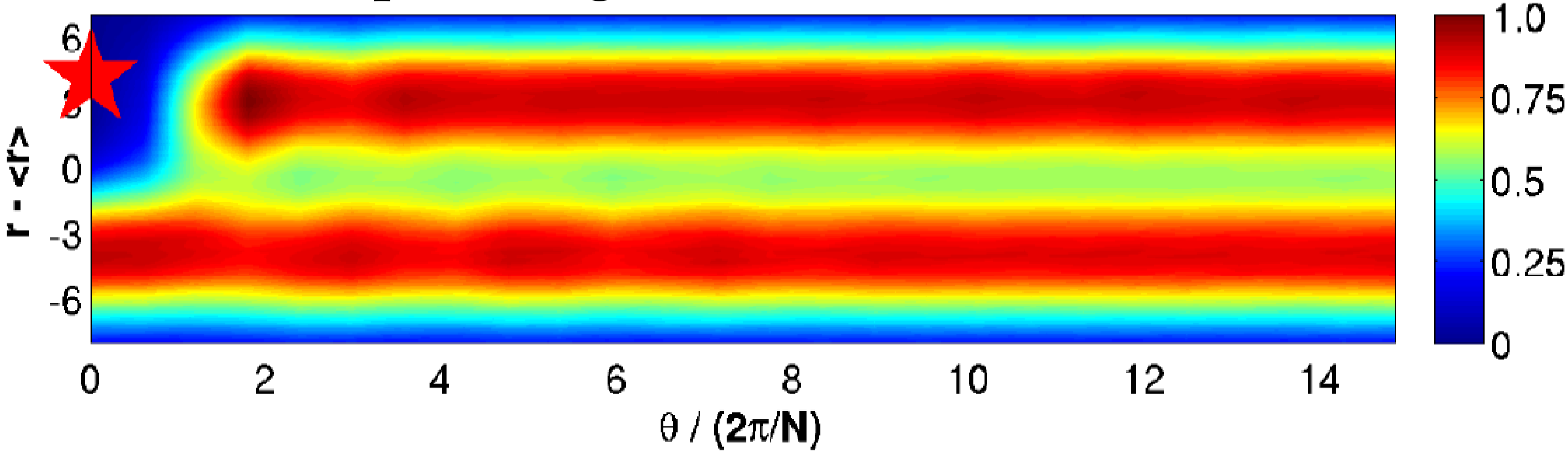


Liquid Regime, ω = 0.1

r_s = **3.0**: Zigzag Regime

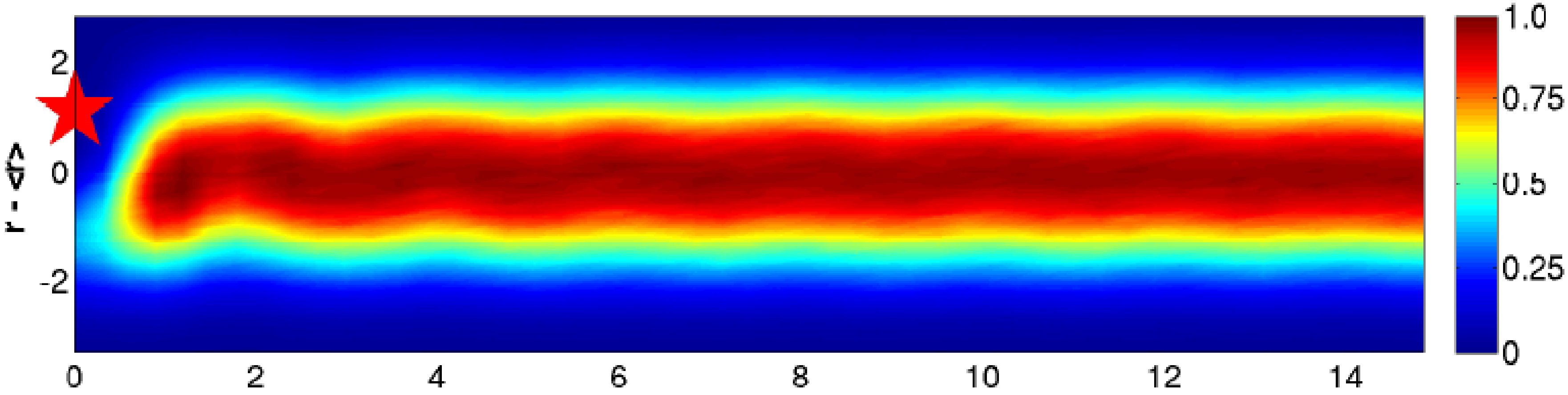


r_s = **2.0**: Liquid Regime (N = 60)

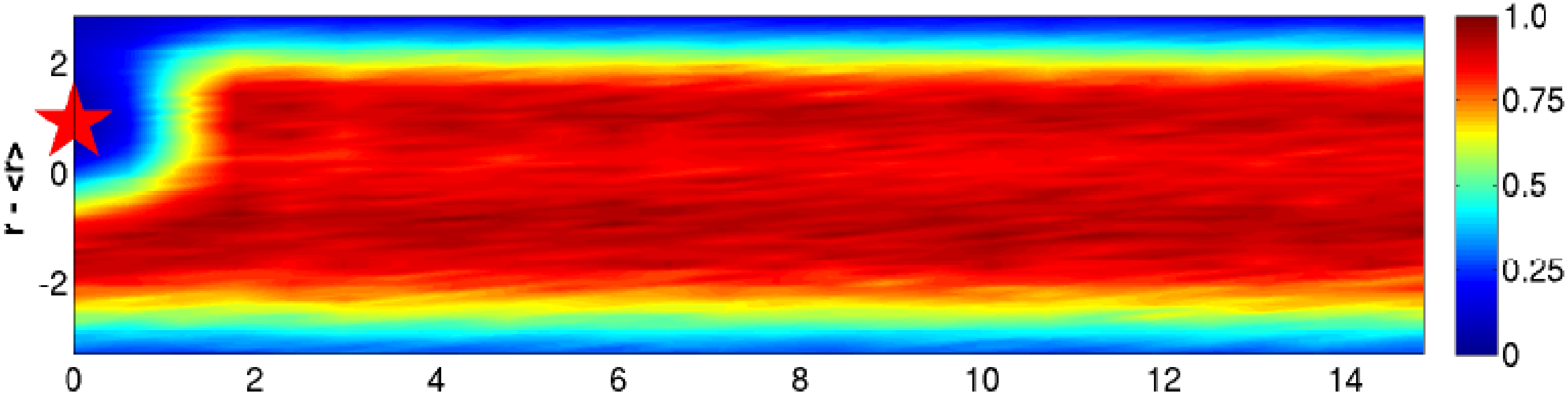


Liquid Regime, ω = 0.6

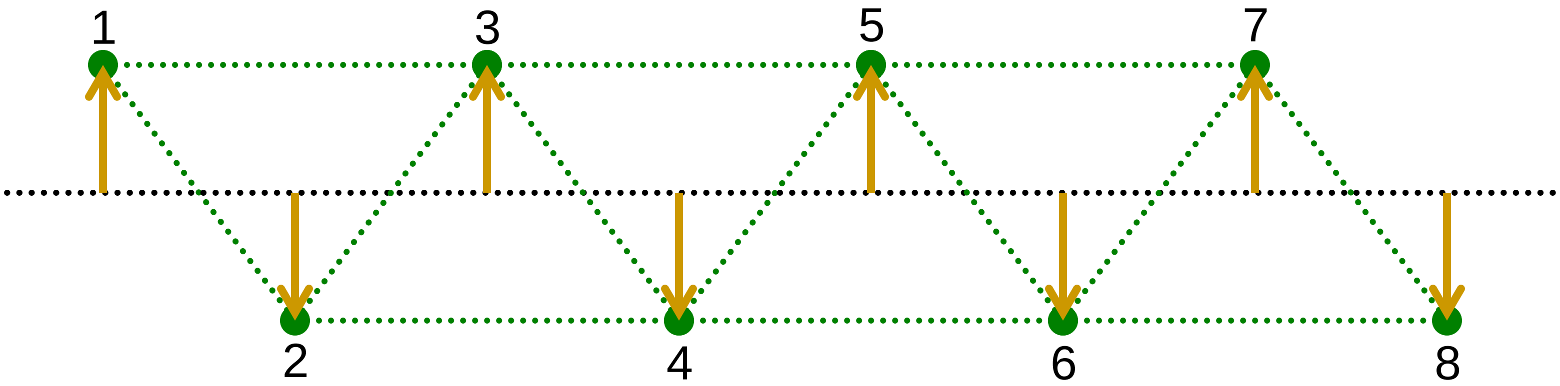
r_s **= 1.3**: Zigzag Regime



r_s **= 0.5**: Liquid Regime (N = 60)



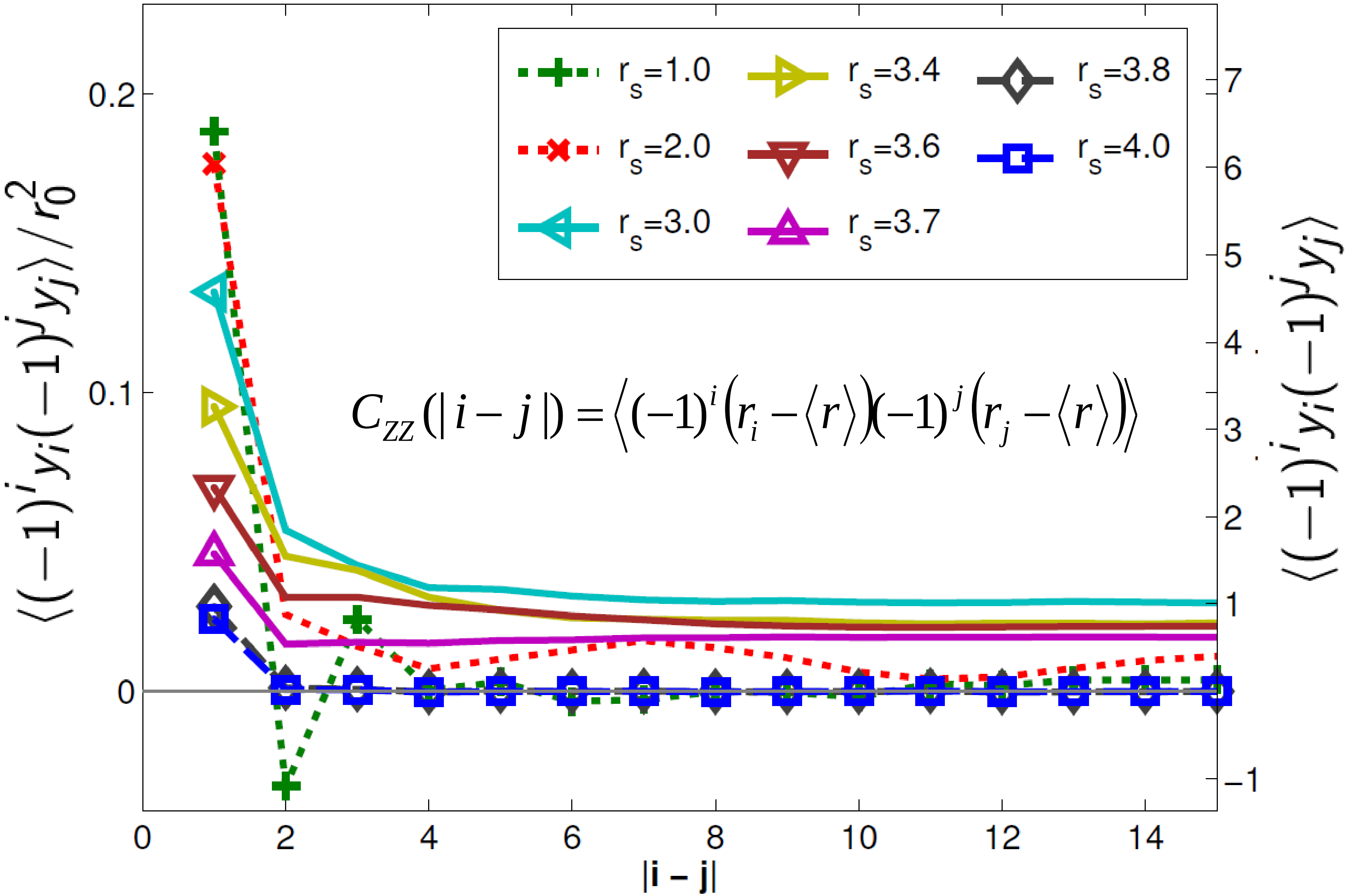
Zigzag Correlation Function, $C_{ZZ}(|i - j|)$



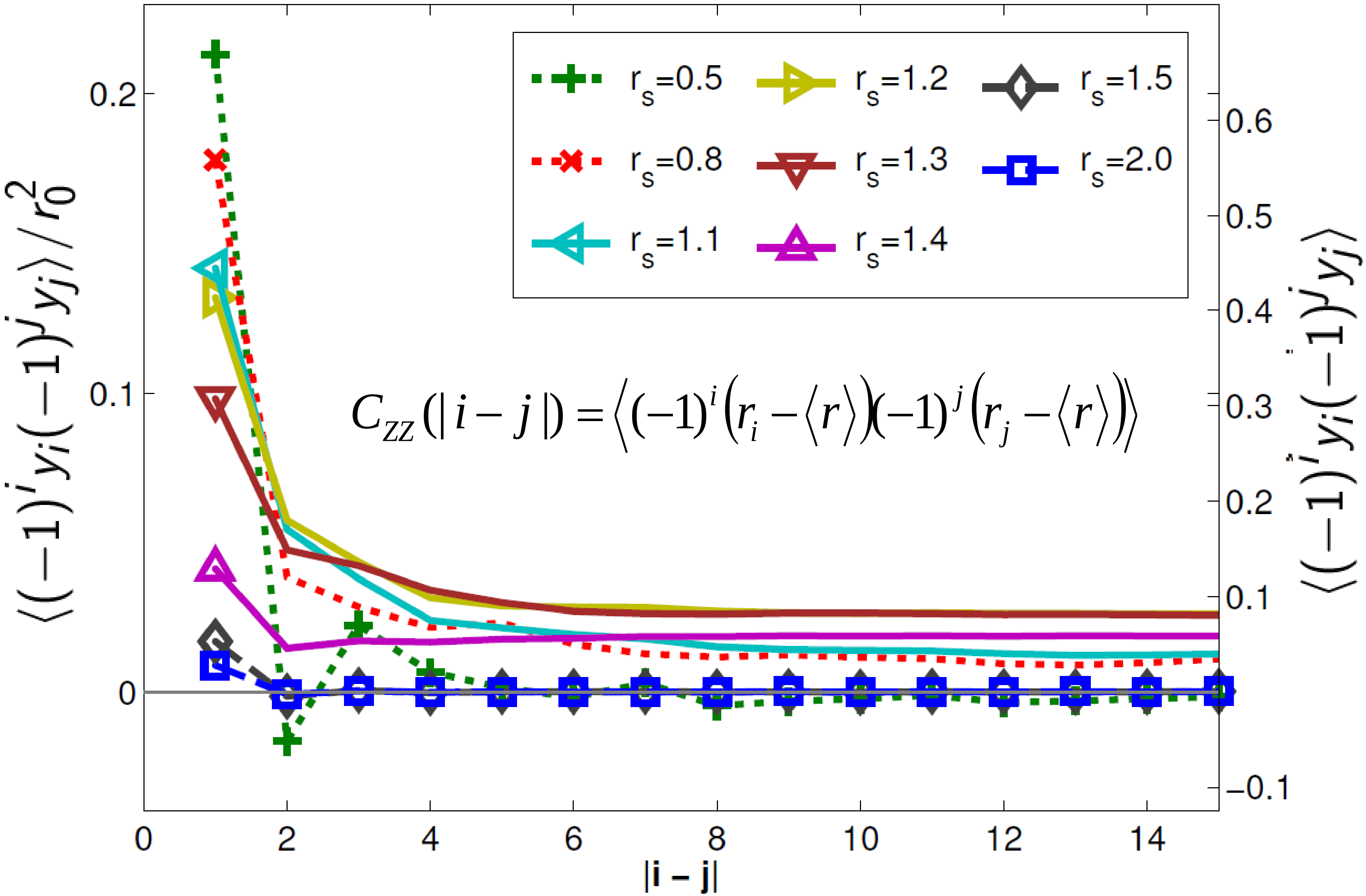
$$C_{ZZ}(|i-j|) = \left\langle (-1)^i \left(r_i - \langle r \rangle\right)(-1)^j \left(r_j - \langle r \rangle\right) \right\rangle$$

- Order electrons along axis of wire
- Zigzag order is not local (tied to coordinate along axis of wire)

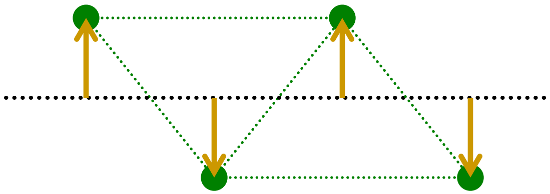
Zigzag Correlation function, ω = 0.1



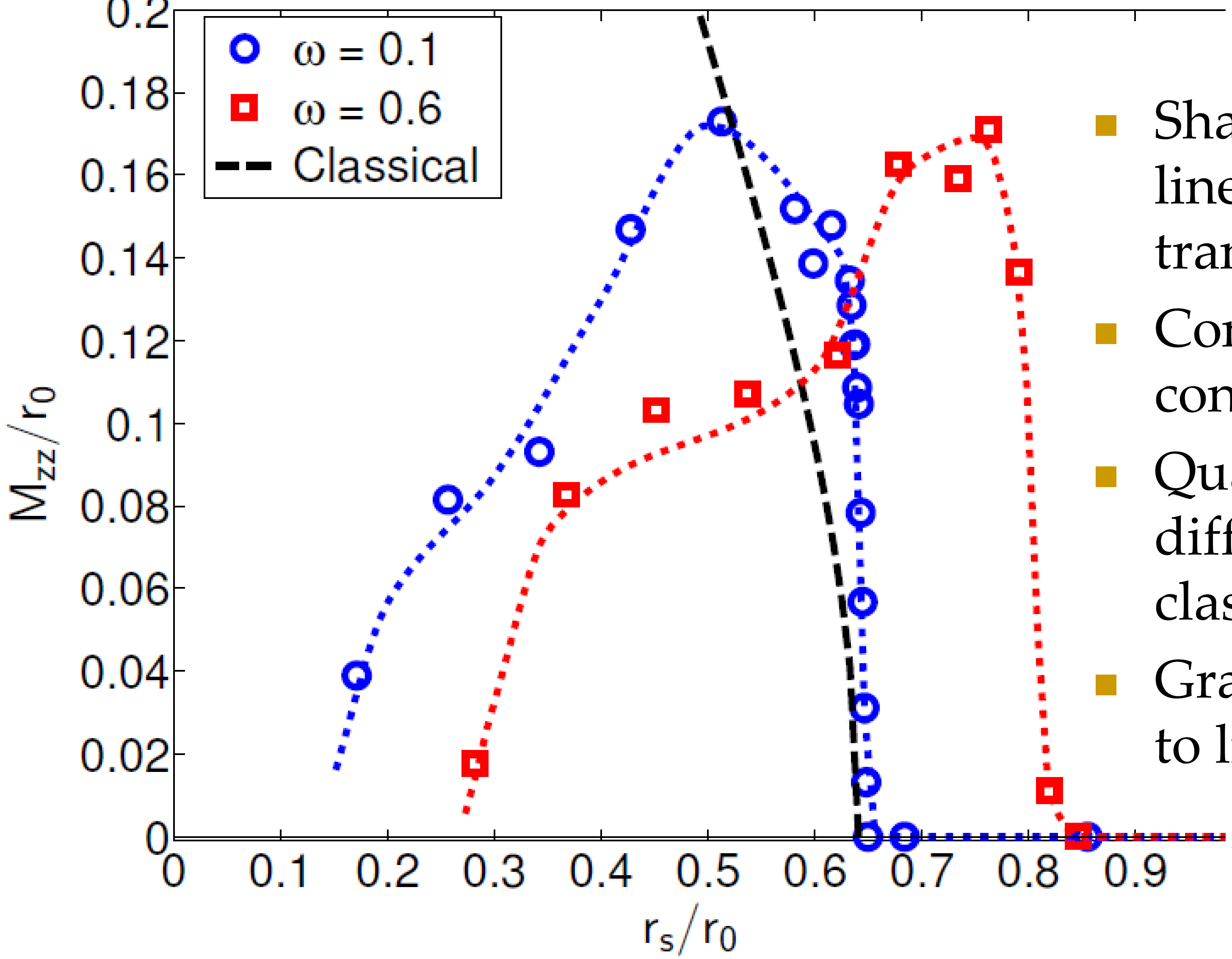
Zigzag Correlation function, $\omega = 0.6$



Zigzag Order Parameter



$$M_{ZZ}^2 \approx \langle C_{ZZ}(|i-j|) \rangle_{|i-j|>N/4}$$



- Sharp increase at linear-zigzag transition
- Consistent with continuous QPT
- Qualitatively different from classical case
- Gradual decrease to liquid regime

Summary: Zigzag

- Zigzag transition occurs at experimentally relevant parameters
- Consistent with continuous quantum phase transition
- Long-range zigzag correlations even when quantum fluctuations smear out pair correlations ($\omega = 0.6$)
- Liquid Phase: Zigzag correlations destroyed

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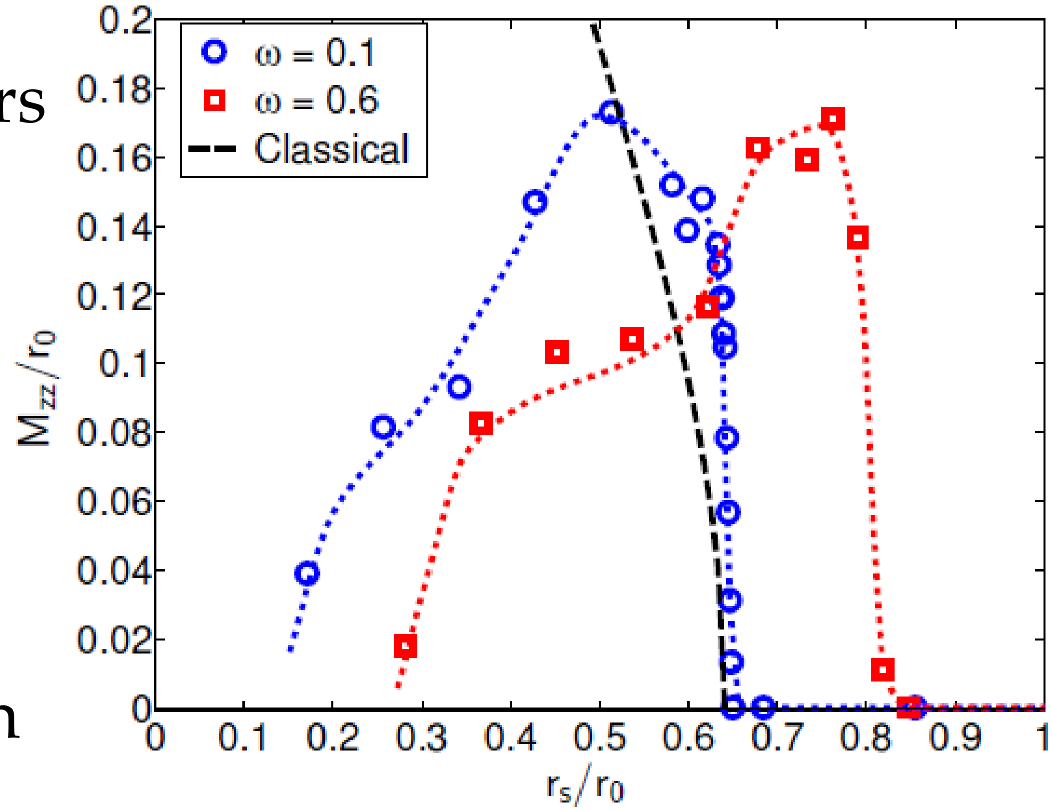
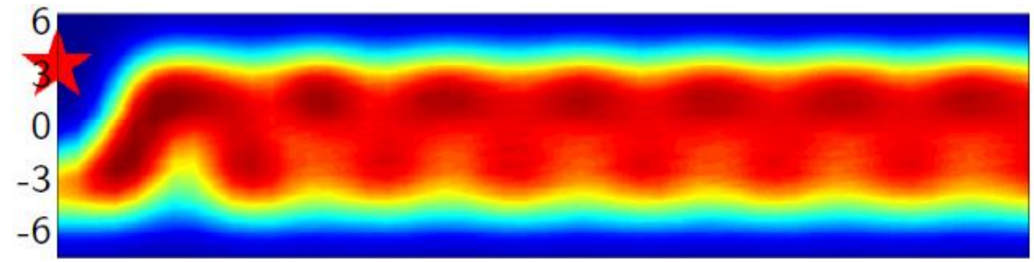
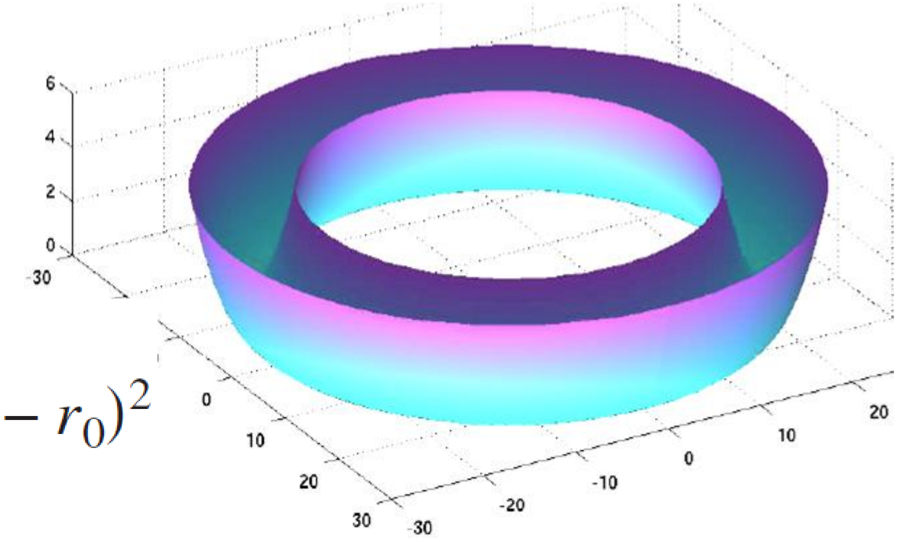




Pair density animations at
http://tinyurl.com/nrbos87

QPC: Model

- N electrons confined to ring with constriction at $\theta = 0$



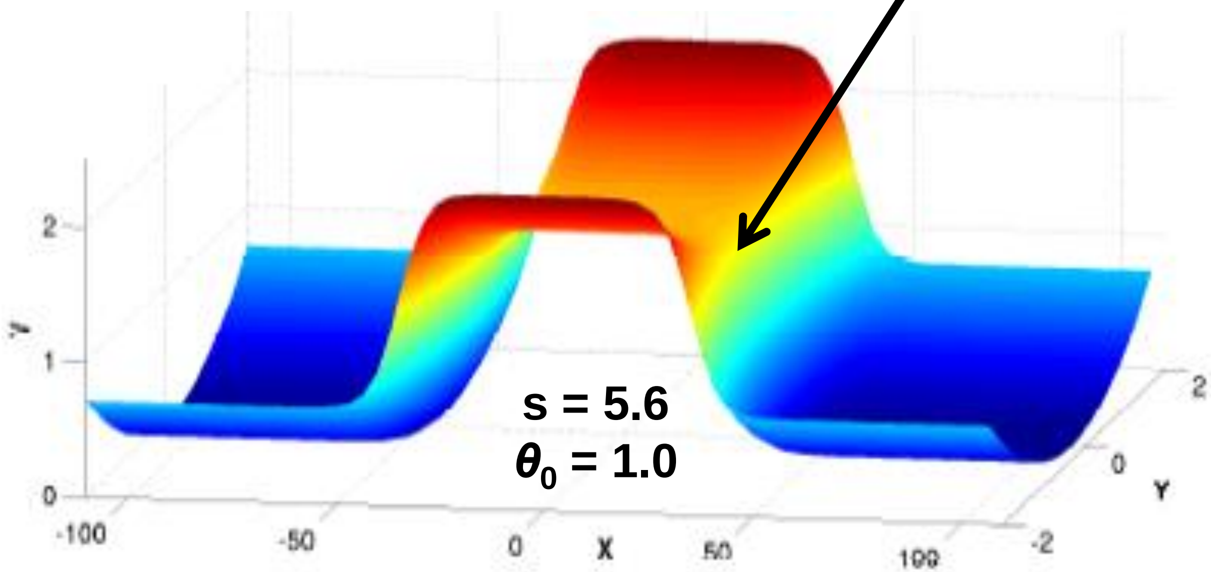
$$H = -\frac{1}{2}\sum_{i}^{N} \nabla_i^2 + \sum_{i<j}^{N} \frac{1}{r_{ij}} + \frac{1}{2}\sum_{i}^{N} \omega^2 (r_i - r_0)^2$$

$$+ V_g\{\tanh[s(\theta_i + \theta_0)] - \tanh[s(\theta_i - \theta_0)]\}$$

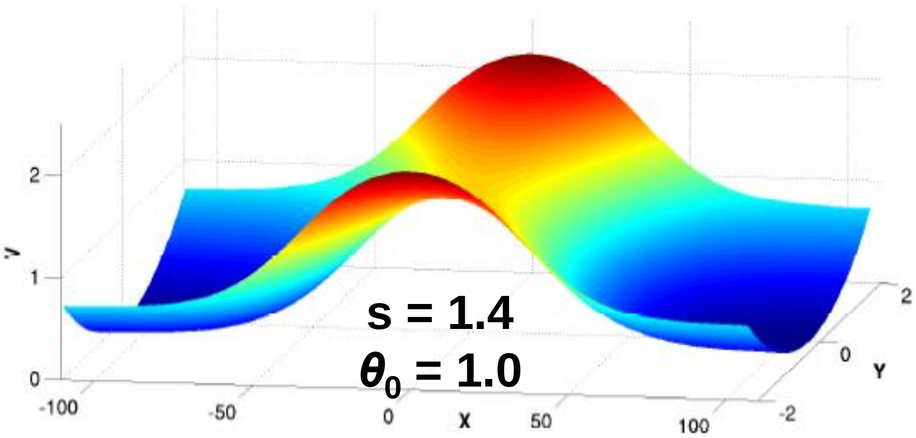
Constriction (QPC)

(or parabolic saddle point)

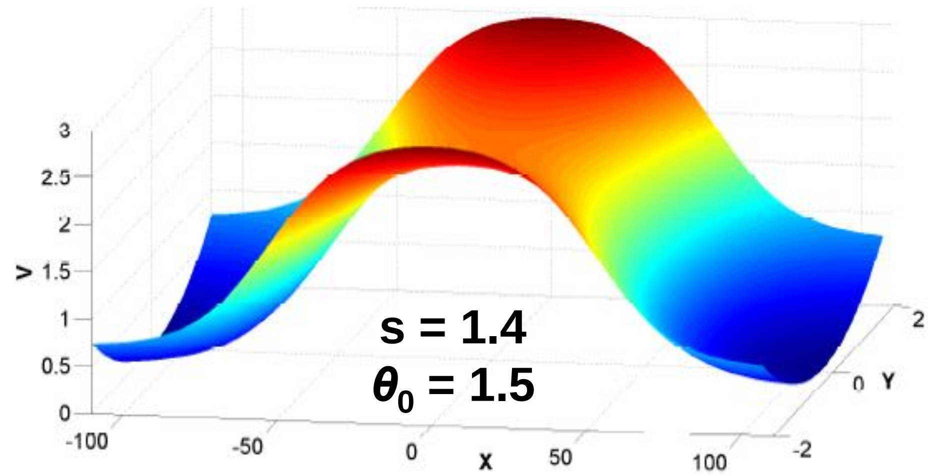
- $\omega = 0.6$, $r_0 = 35$,
  $s = 5.6, 2.8, 1.4$
  $\theta_0 = 1, 1.5$,
  $N = 42, 84, 126$
  (in atomic units)



QPC Model Potentials – Smooth Bump



(c) $V_g = 0.8, s = 1.4, \theta_0 = 1.0$



(d) $V_g = 1.15, s = 1.4, \theta_0 = 1.5$

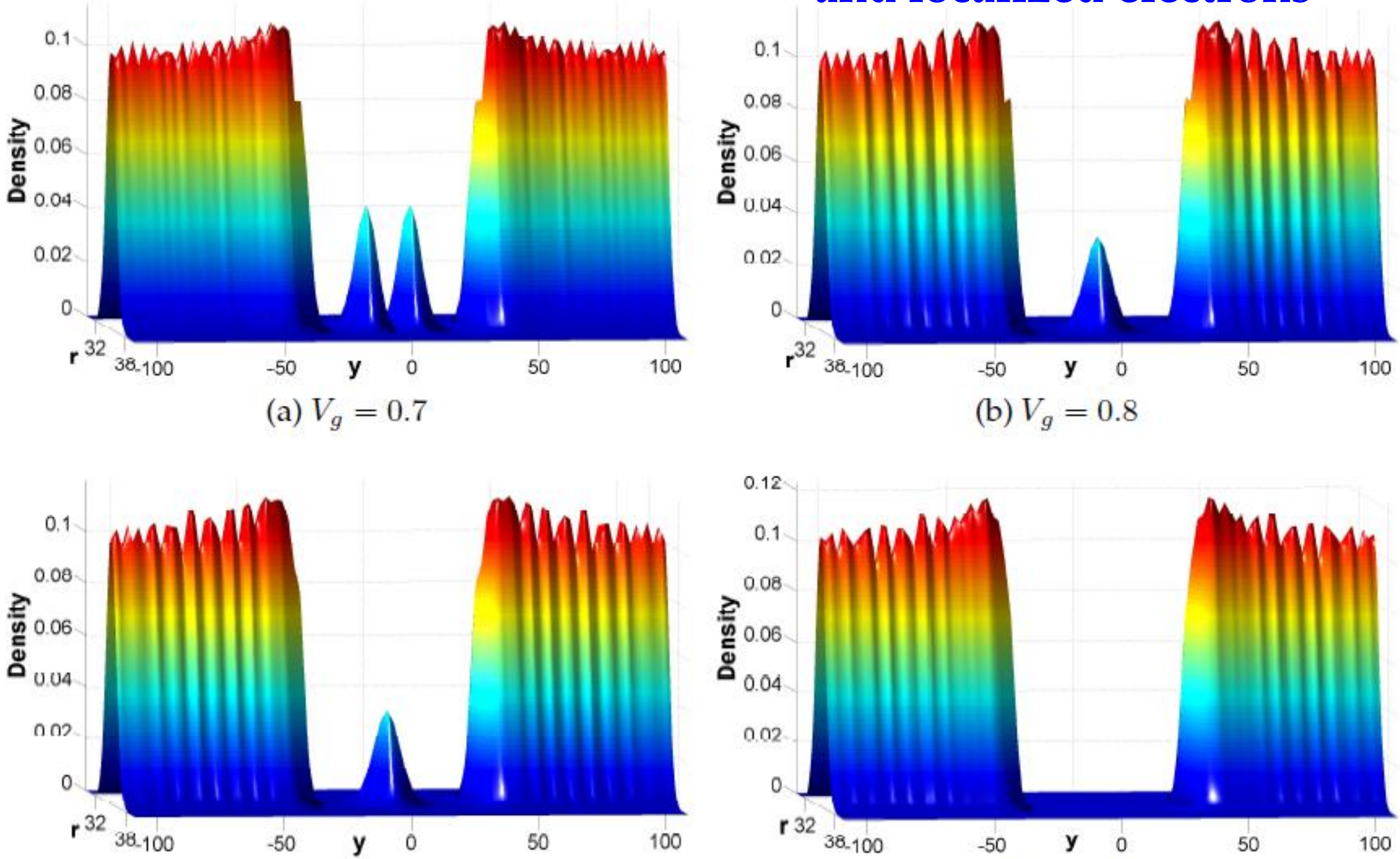
$$V_g\{\tanh[s(\theta_i + \theta_0)] - \tanh[s(\theta_i - \theta_0)]\}$$

- Bump function, s = 1.4, similar to real QPC's
  (Tkachenko et al., J. Appl. Phys, 2001)

Localization in sharp QPC's (s = 5.6)

→Electrons localize in QPC

→Gap forms between leads and localized electrons



(a) $V_g = 0.7$

(b) $V_g = 0.8$

(c) $V_g = 0.84$

(d) $V_g = 0.9$

What causes the gap?

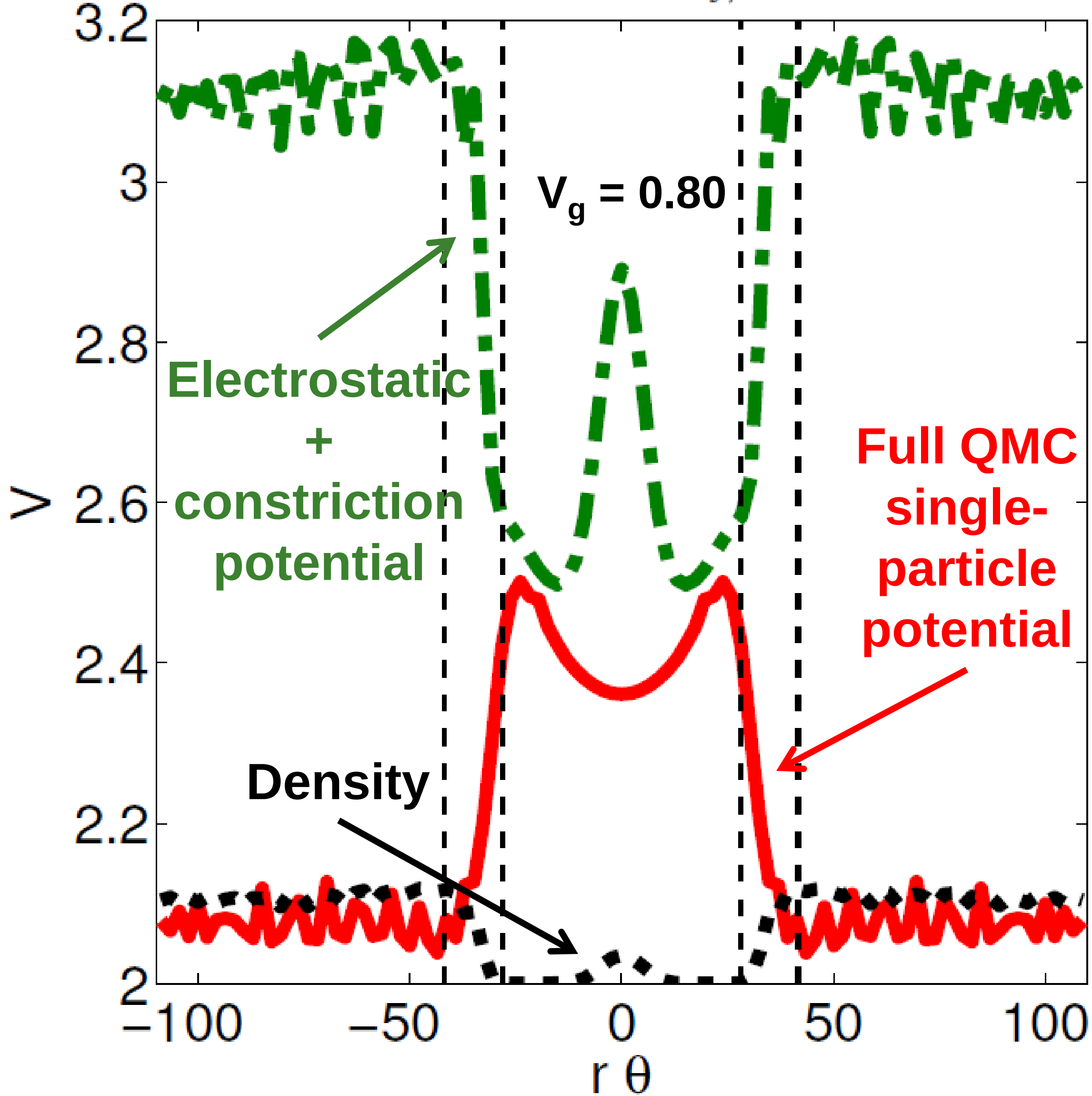
$$V_{1-\text{particle}}(\mathbf{r}) = \frac{1}{n(\mathbf{r})}\int \mathrm{d}\mathbf{r}_1\cdots\mathrm{d}\mathbf{r}_N|\Psi(\mathbf{r}_1\cdots\mathbf{r}_N)|^2\sum_{i=1}^{N}\delta^{(2)}(\mathbf{r}-\mathbf{r}_i)\sum_{j\neq i}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}$$

$$= \frac{1}{n(\mathbf{r})}\int \mathrm{d}\mathbf{r}'\frac{\langle\hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')\rangle}{|\mathbf{r}-\mathbf{r}'|}$$

- Barrier in electronic interaction potential *V(r)* at gap

→**What is the origin of this barrier?**

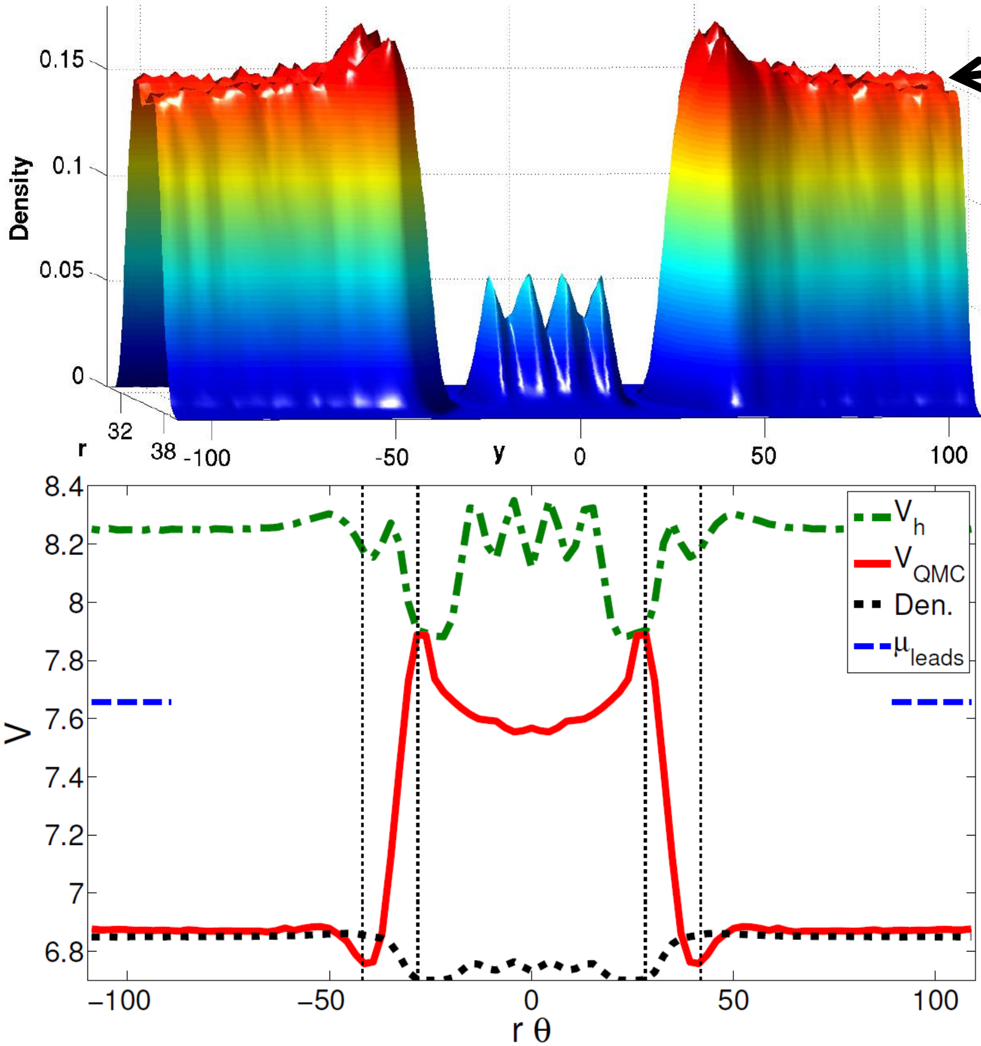
- Simple electrostatics predicts barrier for step
- Our potential (and real QPC's): not that sharp!
- Barrier forms in **exchange-correlation** potential



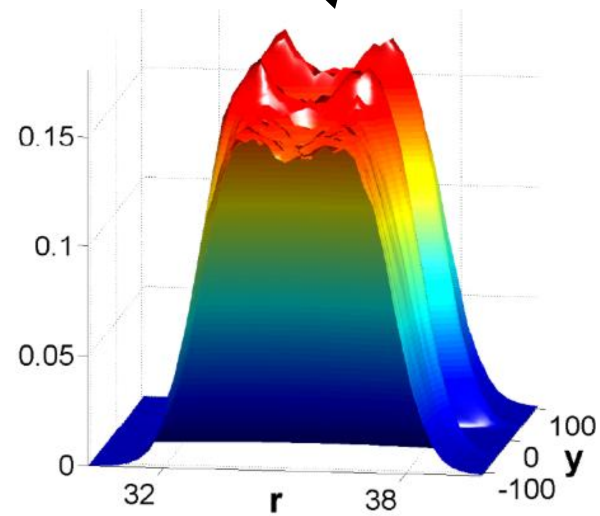
High-Density Leads

N = 126, V_g = 2.5, s = 5.6

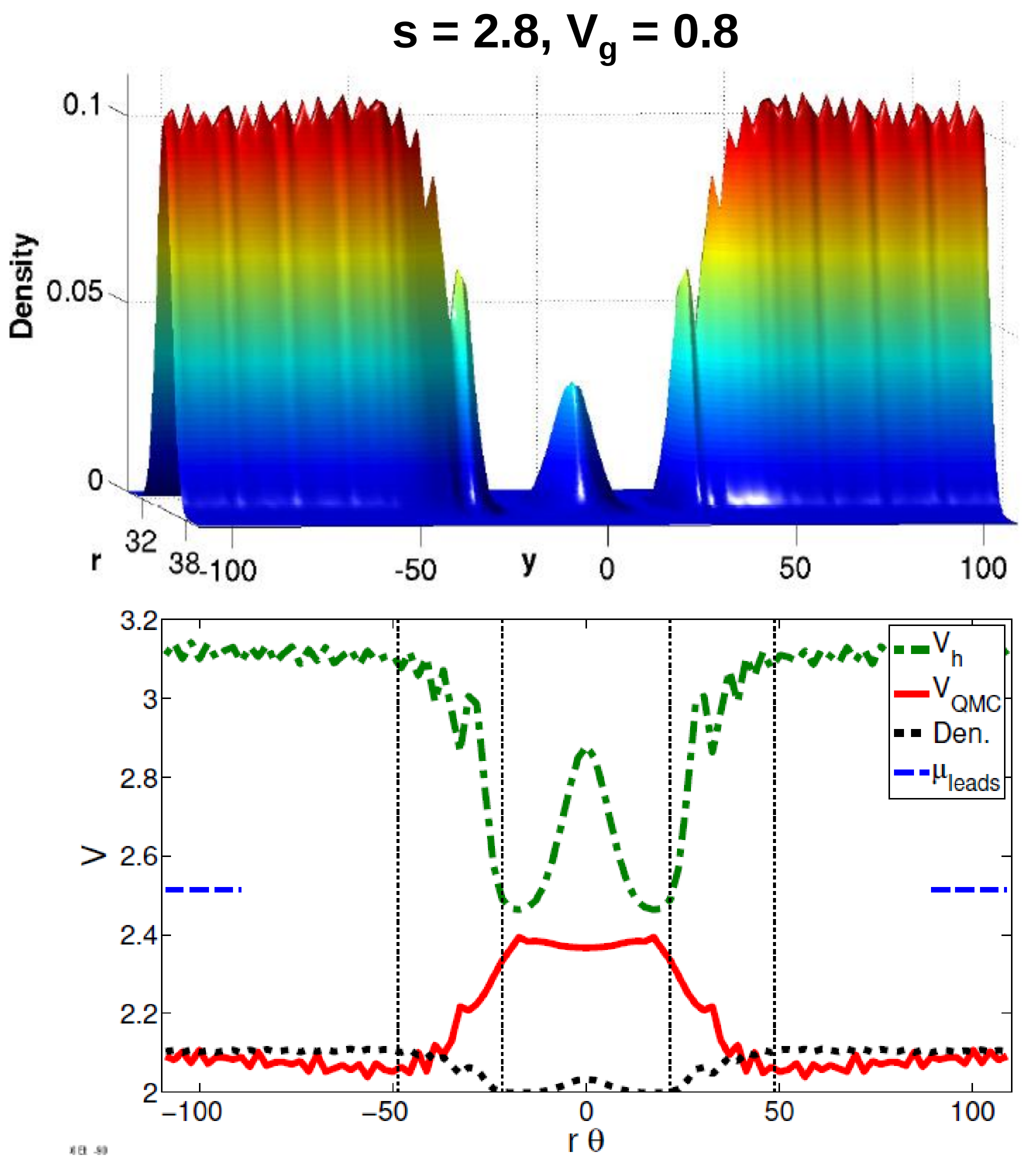
→ Localization, Gap still occur



2 subbands in leads

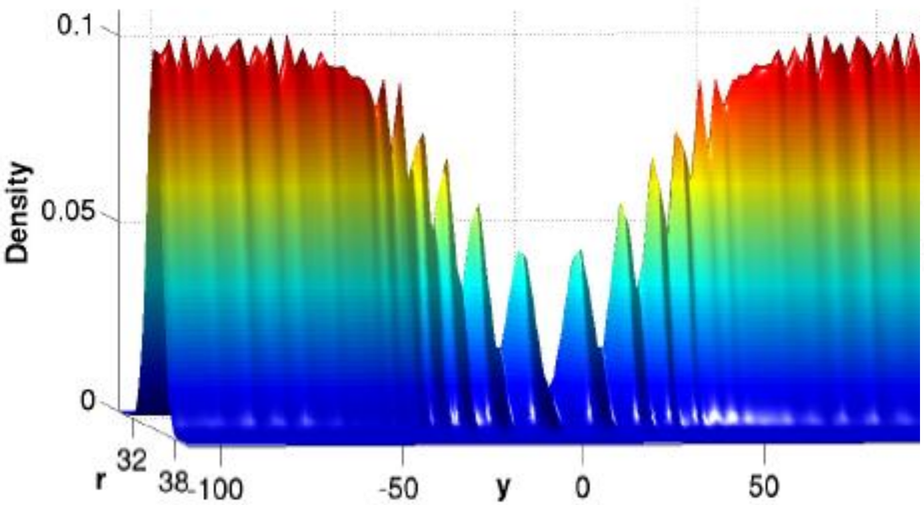


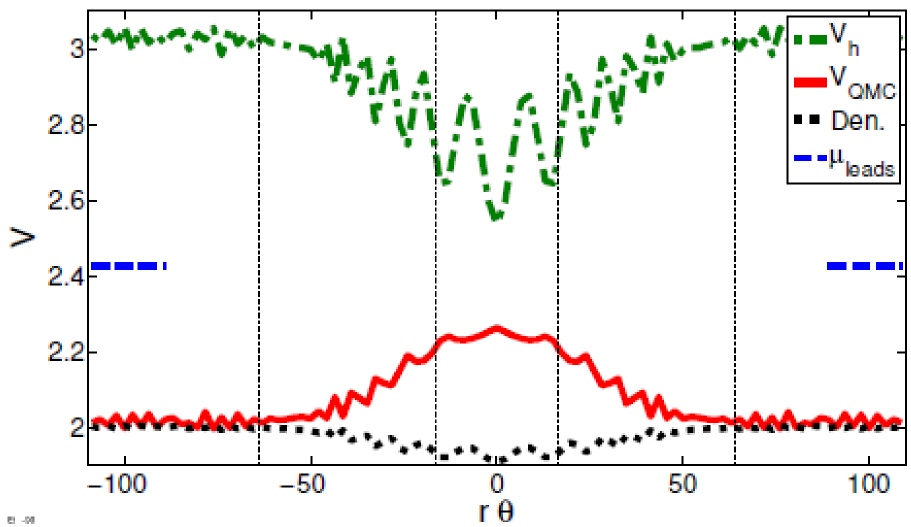
Smooth Constriction Potentials



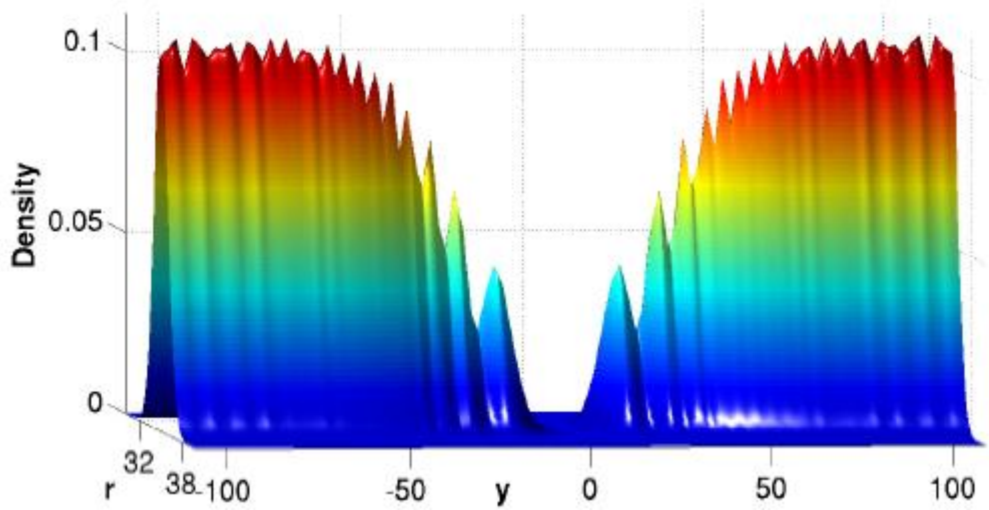
s = 1.4: WC Smoothly Connected to Leads

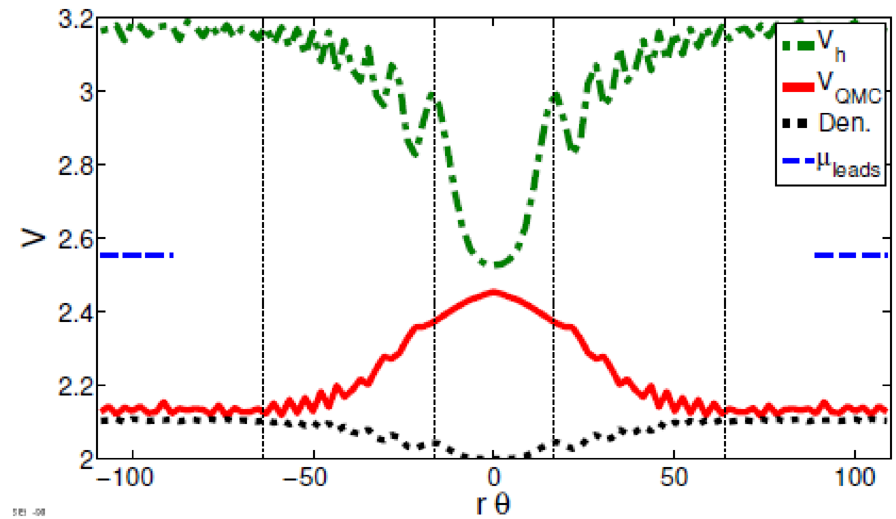
s = 1.4, V_g = 0.75





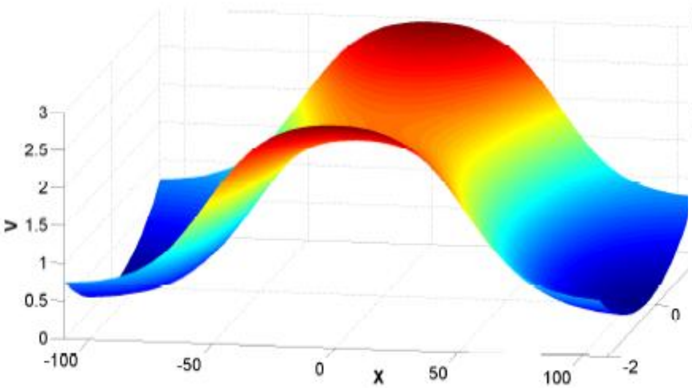
s = 1.4, V_g = 0.92

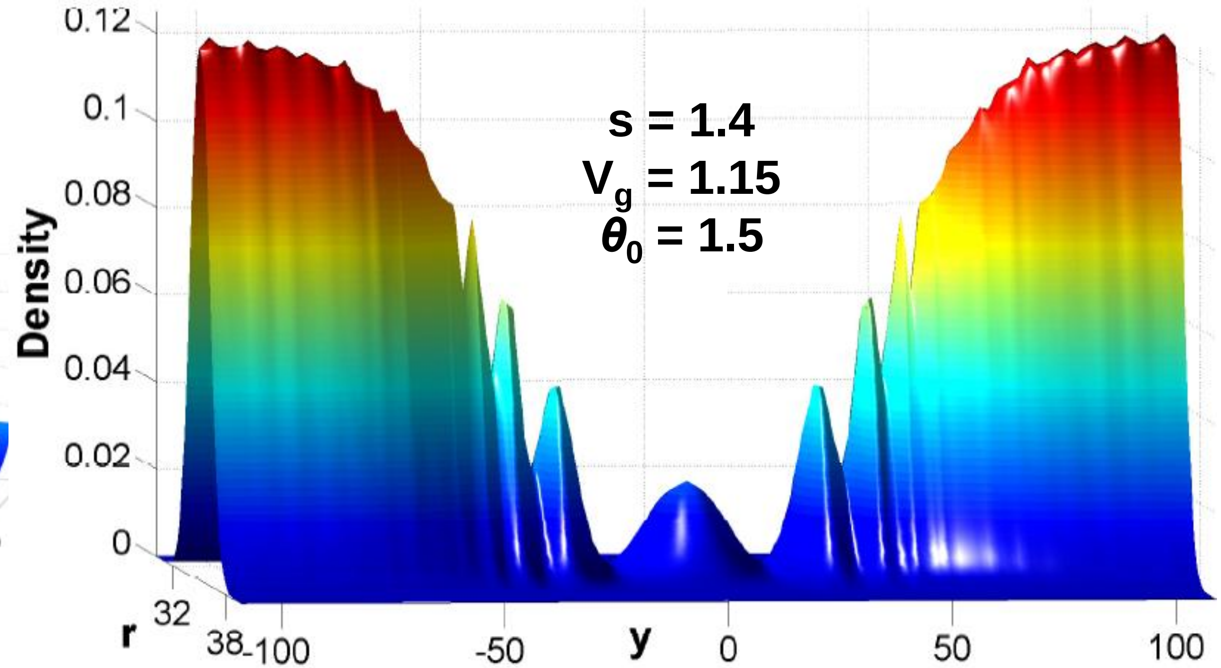




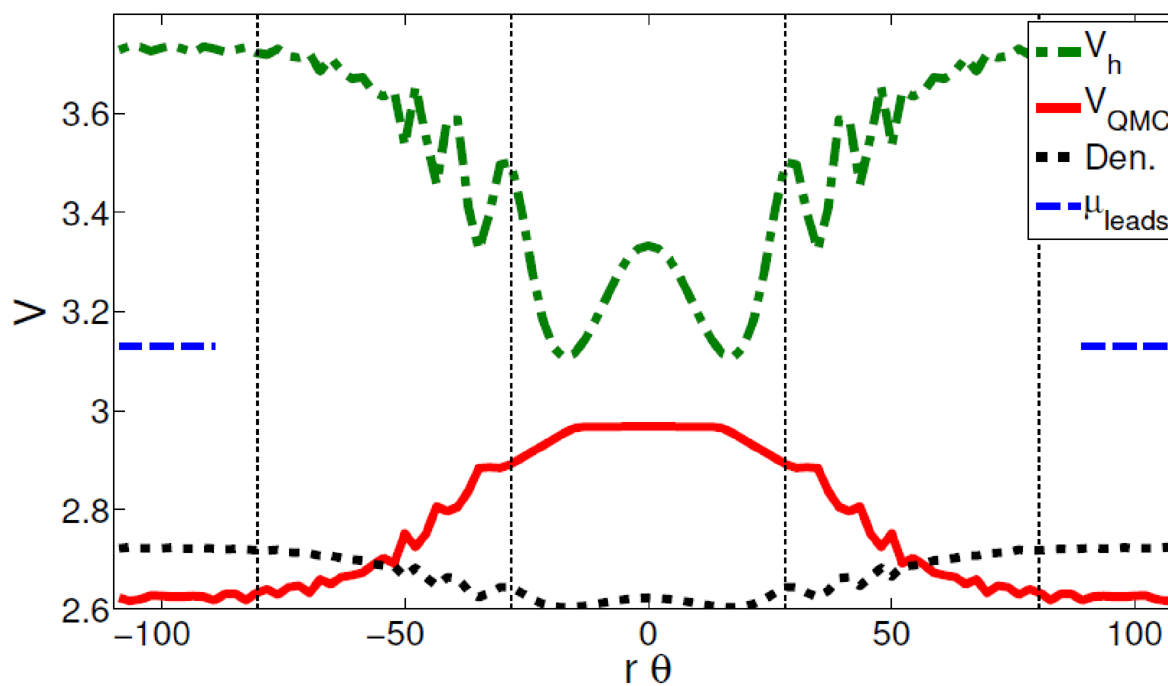
s = 1.4, θ_0 = 1.5

- Long QPC



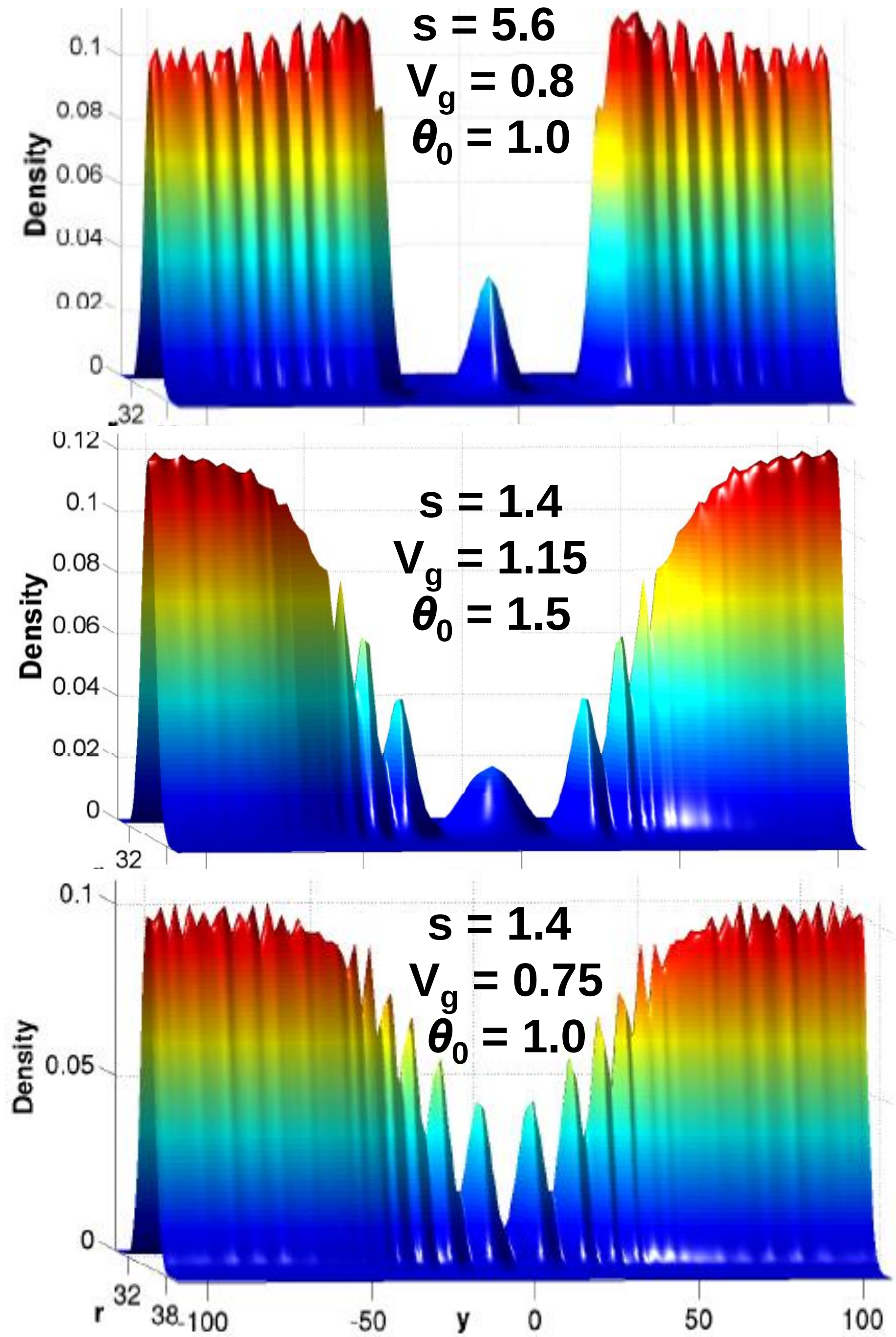


- Isolated state forms in QPC!
- Isolated state can form in smooth QPC if long constriction
- Wigner Crystal in connection region



QPC: Summary

- Isolated state forms for constrictions that have a sufficiently long flat region
  - Localized state detected by e.g. Bird group, Chang group, van der Wal group, …
- Gap in density larger for sharper QPC's
- Wigner Crystal smoothly connects leads to constriction for smoother QPC's
  - Consistent with Matveev 0.7 explanation
- Effects visible for a variety of QPC shapes and with high-density leads



Conclusions

- 1D to Higher-D: Zigzag Transition
  - Consistent with continuous Quantum Phase Transition; qualitatively different from classical case
  - Occurs at experimentally relevant parameters
  - Zigzag order present even in absence of positional order in narrow wires
- Inhomogeneous 1DEG: QPC's
  - Electrons localize in QPC's for a variety of potential shapes due to exchange – correlation
  - Bound state can form even in smooth QPC if long
  - Short, smooth QPC's show WC smoothly connected to leads

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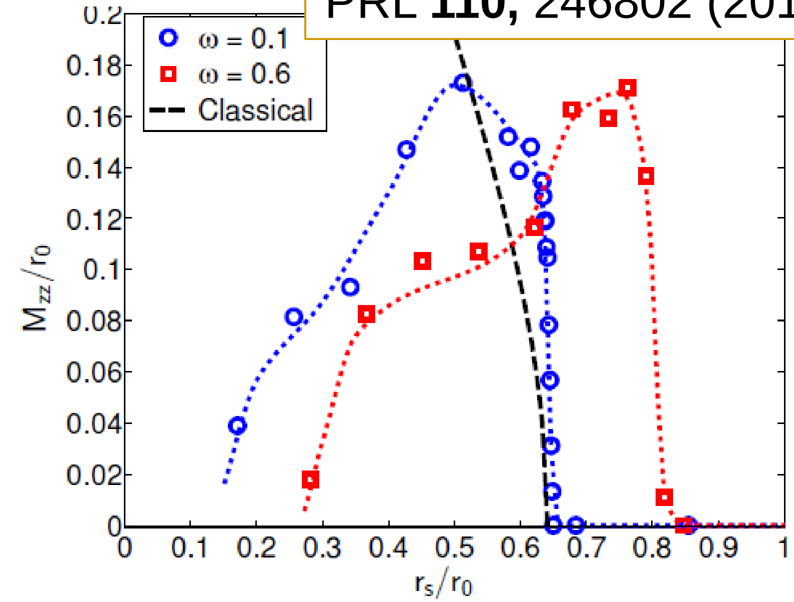

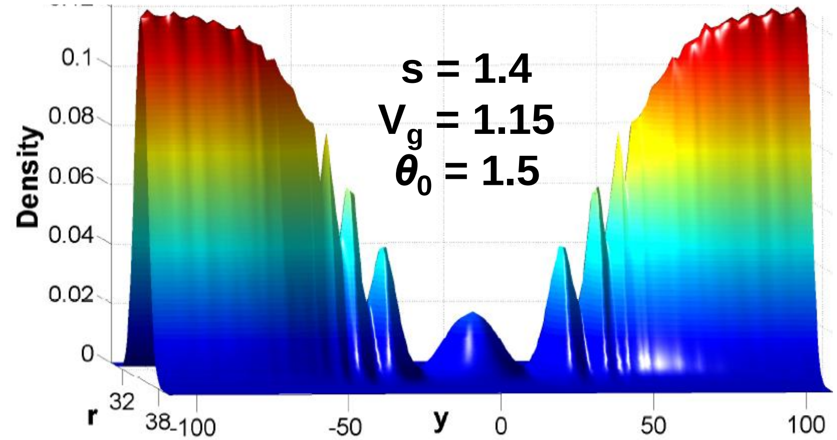

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Supported in part by the DOE