Interaction-Induced Localization in an Inhomogeneous Quantum Wire

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What happens when the density of an electron gas is decreased?

Electrons crystallize! (Wigner, 1934)

Parametrize interaction strength:
\[ r_s^{2D} \equiv \frac{1}{\sqrt{\pi n a_0}} \quad r_s^{1D} \equiv \frac{1}{2n a_0} \]

Extended \[ r_s^c \]

Low density

High density

Localized

Bulk 2D: \[ r_s^c \approx 35 \] (Tanatar and Ceperley ’89, Attaccale et al. ’02, Waintal ‘05)

Intermediate \( r_s \): Complex phases?

Chakravarty, et al. ‘99; Jamei, et al. ‘05; Waintal ‘05
How will such physics appear in an inhomog. or confined system?

1: $n(r)$

- interface between liquid & crystal?
- broken translational invariance $\rightarrow$ smaller $r^c_s$?
- role of interference (mesoscopic fluctuations)?

2: $V(r)$
“0.7 Anomaly” in Conductance of QPC

first pointed out by Thomas et al. (Pepper’s group) PRL1996
Theoretical Themes Concerning the “0.7 Effect”

• Spontaneous spin polarization [many groups]
  “violates” the Lieb-Mattis Theorem:
  ground state in 1D has lowest possible spin
  but system isn’t purely 1D…

• Kondo model [Wingreen & Meir; Rejec & Meir (Nature ‘06)]
  requires a trapped electron in the constriction

• Wigner crystal in the constriction smoothly connected to leads
  [Matveev (PRL ‘04)]
  assumes a smooth connection between effective Luttinger liquids

Is the underlying behavior required by one of these found in an unbiased many-body calculation?
Tunneling Between 1D Wires

Yacoby group (Weizmann) Auslaender, et al. ’02, ’05
Steinberg, et al. ’06
Experiments: Tunneling Between 2 Wires

\[
B^\pm = \frac{\hbar}{ed} |k_F^U \pm k_F^L|
\]

using a fixed, small \(V_{sd}\)

H. Steinberg, et al. (Yacoby group), PRB 73, 113307 (2006)
Experiments: Tunneling Between 2 Wires

\[ B^\pm = \frac{\hbar}{ed} |k_F^U \pm k_F^L| \]

H. Steinberg, et al. (Yacoby group), PRB 73, 113307 (2006)
Model: Quasi-1D Wire with Depleted Region

\[ H = -\frac{1}{2} \sum_{i}^{N} \nabla_{i}^2 + \sum_{i}^{N} V(r_{i}) + \sum_{i<j}^{N} \frac{1}{r_{ij}} \]

\[ V(r) = \frac{1}{2} \omega^2 (r - r_0)^2 + V_{sg}(\tanh(s(\theta + \theta_0)) - \tanh(s(\theta - \theta_0))) \]

- 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: \( N \sim 30 \); size of depleted region \( \sim 0.3-0.7 \) \( \mu \text{m} \) for GaAs
 VM C followed by DMC with fixed node approximation

based on variational principle:

\[ E_{VMC} = \frac{\int \Psi_T^*(R) \mathcal{H} \Psi_T(R) dR}{\int \Psi_T^*(R) \Psi_T(R) dR} \geq E_{GS} \]

trial wave-function:

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

Jastrow part, \( J = \prod_{i<j} \exp \{ a_{ij} / (1 + b_{ij}) \} \)

\( \Rightarrow \) 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

$V_{gs} = 0.2$

$N = 30, S = 0, L = 0.35$

$V_{gs} = 0.3$

$V_{gs} = 0.4$

$V_{gs} = 0.5$

$\rho (r, \theta) \times 10^3 \, \mu m^{-2}$

$r [\mu m]$
Density

N=30, L=0.3

S=0, up+dn

S=2, up

excited state with S=2

electron in depleted region very polarized

S=2, dn
Density: Long Constriction, Steepness of Potential

- **Potential A**: steep external potential
- **Potential B**: steep external potential
- **Potential C**: smooth external potential
- **Potential D**: smooth external potential

**N=31, L=0.7**
Density: Long Constriction, Steepness of Potential

- **Potential A**: steep external potential
- **Potential B**: gap develops between liquid and crystal !!!
- **Potential C**: smooth external potential
- **Potential D**: 

\[ N=31, \; L=0.7 \]
Depleting a Long Constriction

Potential B
N=31

- density modulation indicating start of localization at $r_s \sim 3.5$
- gap between localized and liquid parts starts at $r_s \sim 5.5$
- gap $\rightarrow$ Coulomb blockade $\rightarrow$ number in depleted region changes abruptly
Comparison of Different Methods

QMC with either gaussian or LSDA orbitals in the trial wavefunction: in close agreement for energy and density → can use either, makes no difference
Spin Structure: Pair Density

Pair density: fix an up electron – marked by the black arrow
Shown: [n(r) of up electrons] – [n(r) of down electrons]

N=31, L~0.7

Looks like an antiferromagnetic state in the depleted region
Spin Gap: Ferro vs. Antiferro

Difference between energy of fully polarized state and antiferromagnetic state

**Uniform ring:**

Fully polarized state is always higher in energy

**Inhomogeneous ring:** (ie. with depletion region)
Thomas-Fermi Densities

Gap between two regions present to some extent in TF treatment
→ gap is partly electrostatic in origin
Circular Quantum Dot

How will such physics appear in a confined system?

- inhomogeneous electron density – boundary between liq. & xtal?
- broken translational invariance $\rightarrow$ smaller $r_s^c$?
- mesoscopic fluctuations (i.e. interference effects)?

**Model:**

- Kinetic Energy $\left(-\frac{1}{2}\nabla^2\right)$
- Coulomb Repulsion $\left(\frac{1}{|r_i - r_j|}\right)$
- Confinement Potential $\left(\frac{1}{2}\omega^2 r^2\right)$

**parabolic confinement – circular symmetry**

Spring constant $\omega$ controls $r_s$.

Range: $3 > \omega > 0.001$ ($0.4 < r_s < 60$) for $N$ up to 20
Density of Electrons: $n(r)$

$N=20$
$L=0, S=0$

$\rho_s = 0.41$
$(\omega = 3.0)$

$\rho_s = 4.7$
$(\omega = 0.06)$

$\rho_s = 9.5$
$(\omega = 0.02)$

$\rho_s = 14.7$
$(\omega = 0.01)$

3 rings as in classical limit

sharp rings form! – dot is bigger for larger $\rho_s$

[Amit Ghosal]
Pair Density

\[ g_{\sigma \sigma'}(r_0; r) \]

The probability of an electron with spin \( \sigma' \) at \( r \) given an electron with spin \( \sigma \) fixed at \( r_0 \)

\[ r_s \approx 0.4 \]

\( N=20: L=S=0 \)

\[ r_s \approx 15 \]

[Amit Ghosal]
Pair Density: High $r_s$

$N=18$: $L=3$, $S=9$ (fully polarized)

$r_s \approx 50$

electrons form sharp peaks – crystal-like!

[Devrim Güçlü]
Evolution of Rings in $n(r)$

Characterize the strength of the ring structure by "fractional peak height" (FPH):

Development of FPH is completely smooth – no threshold

[Amit Ghosal]
Magnitude of Angular Modulation: Power Spectrum

Find the power spectrum in the $\theta$ direction at each $r$:

$$f(r, k_\theta) = \frac{2}{r^2} \int dr_1 \ldots dr_N |\Psi(r_1, \ldots, r_N)|^2 \sum_{i<j}^N \cos[k_\theta (\theta_i - \theta_j)] \delta(r_i - r) \delta(r_j - r)$$

$r_s \approx 5$

$r_s \approx 50$

N=18: L=3, S=9 (fully poalized)

[Devrim Güçlü]
Development of Peaks in Power Spectrum

Height of the principal peak in the **angular power spectrum** as a function of $r_s$

- completely smooth! – no special value of $r_s$
- similar curve for $N=19$ outer and inner ring
Development of Peaks in Power Spectrum (2)

Can have several peaks in power spectrum – superposition of states with different number of particles in the ring

\[ N=6, \; L=0 \]

\[ k_\theta=5 \]

\[ k_\theta=6 \]
Tool for Observation: Coulomb Blockade

**Isolated dot:** $Q$ quantized

\[
U(N) = \frac{1}{2} \frac{e^2 N^2}{C} - e V_g N \left( \frac{C_g}{C} \right) = \frac{e^2 (N - N_g)^2}{2C} ; \quad N_g \equiv \frac{C_g V_g}{e}
\]

![Diagram showing the potential energy $U$ as a function of $V_{gate}$ with $N$, $N+1$, and $N+2$ labeled.]
Coulomb Blockade Peak Spacing

- weakly coupled leads: $Q$ jumps sharply $(G_{L,R} \ll \frac{e^2}{h}; T \ll \frac{e^2}{C})$
- $Q$ jumps and $G$ has peak when:

\[
E_{gr}(n) - \frac{C_g}{C} e n V_g^* = E_{gr}(n + 1) - \frac{C_g}{C} e (n + 1) V_g^*
\]
Coulomb Blockade: Classical vs. Quantum

Classical:
- position: constant spacing $= \frac{e^2}{C}$
- peak height: constant given by series resistors $G_{\text{peak}} = \frac{G_1 G_2}{G_1 + G_2}$

Quantum:
- position: single particle energies and residual interactions $\rightarrow$ spacing fluctuations
- peak height: coupling from quantum state $\psi$ in dot to lead $\rightarrow$ height fluctuations
Vertical Quantum Dots

(a) Schematic diagram of a vertical quantum dot with a side gate, drain, and source. The approximate size is 0.5 µm. 

(b) Cross-sectional diagram showing the dot and AlGaAs, InGaAs, and n-GaAs layers.

(c) Images of different quantum dots with varying shapes and sizes. 

Experimental Coulomb Blockade – Vertical Quantum Dot

[Diagram showing a nanoscale device with labels for Drain, Dot, Side gate, Source, and layers of AlGaAs and InGaAs.]

CURRENT (pA)

Addition energy (meV)

N=0 2 6 12 16

GATE VOLTAGE (V)

0 1.5 -0.8

Addition Energy: Coulomb Blockade Peak Spacing

\[ \Delta^2 E(N) = E_G(N + 1) + E_G(N - 1) - 2E_G(N) \]

Classical structure develops for small \( N \rightarrow \) localization!

\( r_s \) (approx)

Shell effects

fully polarized case

[Devrim Güçlü & Amit Ghosal]
CONCLUSIONS

Interaction-Induced Localization in
1. Inhomogeneous Quantum Wire, 2. Circular Quantum Dot

- "High-Low-High" structure (quasi-1D)
  - low density $\rightarrow$ stronger interactions $\rightarrow$ localization
  - nature of interface controlled by steepness of potential
  - gap can form between crystal and liquid $\rightarrow$ C. blockade effects
  - short constriction: single electron trapped, barrier is dynamic
do Kondo correlations form?

- Circular Parabolic Quantum Dot
  - rings form first, then angular modulation -- both smooth
  - interactions act on pre-existing modulation caused by interference
  - use conductance CB peaks to observe transition

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