Persistent current and Wigner localization in a one-dimensional quantum ring

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Introduction

Experimental situation

- Effectively one-dimensional system can be realized experimentally
- Number of electrons can be controled in these gated semiconductor heterostructures
- Allows to study many-body effects (electronic interaction) in these systems

Low-density limit: Wigner crystal

- For very low densities: Coulomb energy dominates the system
- Localization of electrons as an electron crystal: Wigner crystal

Theory

Search a measure for the localization of an electronic state

Outline

Indirect localization criteria

Spatial extension of the wave function

Inverse participation number is a measure of the region in space where the wave function significantly differs from zero

- Inverse participation number of a single particle state

$$P^{-1} = \frac{\int d^3r \, |\varphi(\vec{r})|^4}{\left[\int d^3r \, |\varphi(\vec{r})|^2\right]^2}$$

- Generalization for Density Functional Theory

$$P^{-1} = \frac{\int d^3r \, (\rho(\vec{r}))^2}{\left[\int d^3r \, \rho(\vec{r})\right]^2}$$

The larger the inverse participation number, the more localized is the state

Indirect localization criteria

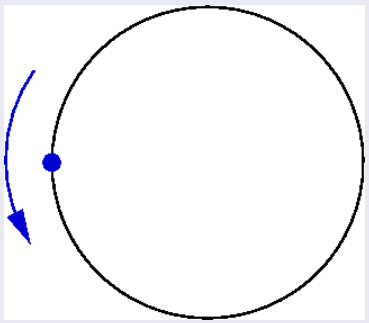
Curvature of the ground-state energy

- Idea: Extended (delocalized) state is sensitive for the boundary conditions in a large system, a localized state not
- How does the ground state energy change as a function of the boundary conditions?
- Consider the curvature of the ground state energy with respect to the boundary conditions:
  - Extended system $\longrightarrow$ sensitive to the boundary conditions $\longrightarrow$ large value for the curvature
  - Localized system $\longrightarrow$ insensitive to the boundary conditions $\longrightarrow$ small value for the curvature

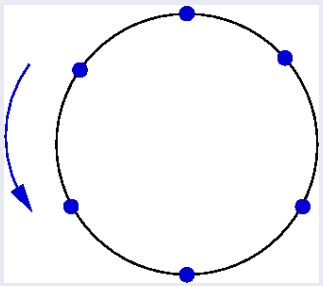
Direct localization criterion: current

Persistent current of a delocalized system

- Non-interacting particles: total current is a sum of the currents of individual particles



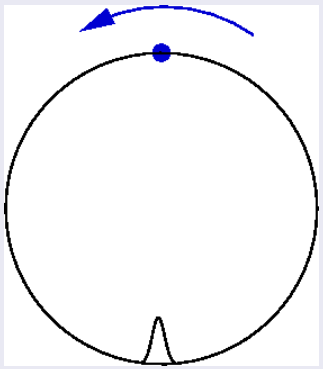
- Interacting particles in a clean sample behave as non-interacring particles concerning the persistent current



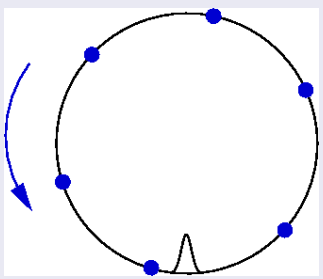
Direct localization criterion: current

Persistent current of a localized system

- Single particle in a system with impurity: Current dictated by single particle tunneling



- Interacting particles: Correlated system tunnels as a whole



- This means: persistent current is suppressed by the interaction

One-dimensional Wigner crystal

One-dimensional electron gas

- Kinetic energy per particle

$$\frac{T}{N} = \frac{L}{2\pi N} \int_{-k_F}^{k_F} \frac{\hbar^2 k^2}{2m^*} dk \propto n^2$$

- Coulomb energy per particle

$$\frac{V}{N} \propto \frac{1}{d} \propto n$$

Wigner transition at a critical density

- High density: Free electron gas-like behaviour since $T \gg V$
- Low density: Localization of electrons since $V \gg T$

Stability of a 1D Wigner crystal

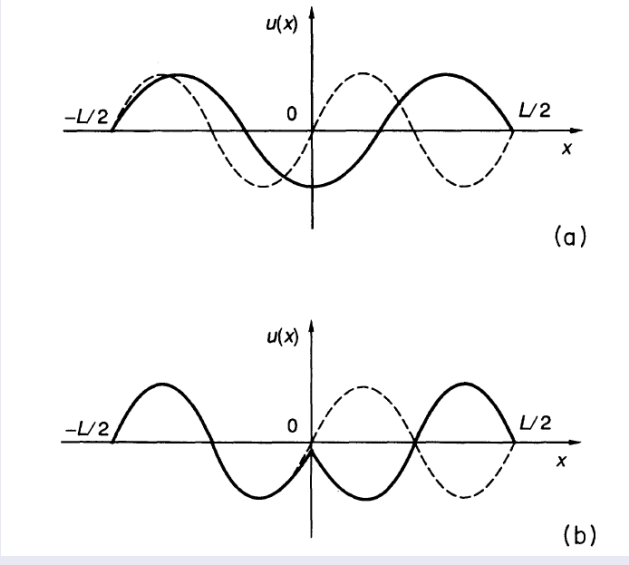
Quantum fluctuations

- Consider a 1D Wigner crystal as a chain of electrons connected by springs
- Quantum mechanical zero-point oscillations of the normal modes of this chain lead to fluctuating displacements of the electrons
- Long wavelength fluctuations (small k) lead to a divergency of the expectation value of the squared displacement
- Should be no crystalline order in 1D

Stability of a 1D Wigner crystal

Pinning

- Idea: Pinning potential suppresses long wavelength modes (soft modes) by creating a node for these modes at the impurity potential site[a]

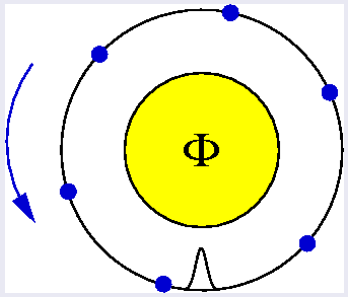


- No divergency of the fluctuations $\Rightarrow$ 1D Wigner crystal stabilized

[a] L.I.Glazman et.al., Phys.Rev.B **45**, 8454 (1992)

Model

One-dimensional quantum ring



One-dimensional N-particle system of length L with periodic boundary conditions

Hamiltonian

$$\hat{H} = \sum_{i=1}^{N} \left[\frac{1}{2m^*} \left(-i\hbar \frac{d}{dx_i} - eA \right)^2 + V_{\mathrm{imp}}(x_i) \right] + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|x_i - x_j|}$$

with

- Vector potential $A = \frac{\Phi}{L}$ induces a persistent current
- Gaussian impurity V_{imp} pins the Wigner crystal

Model

One-dimensional Wigner-Seitz radius r_S

Ratio between Coulomb and kinetic energy: $\frac{\langle V_C \rangle}{\langle T \rangle}$:

$$r_S \propto \frac{1}{N}\frac{L}{a_B} \quad (\text{dimensionless parameter})^a$$

with the Bohr radius

$$a_B = \frac{\epsilon \hbar^2}{m_0^* e^2}$$

In GaAs ($\epsilon = 12.5$, $m_0^* = 0.0665 m_e$): $a_B = 9.95 \cdot 10^{-9}$m

[a] Markus Hofmann, PhD thesis, Universität Erlangen-Nürnberg (2005)

Changing r_S from $r_S \ll 1$ to $r_S \gg 1$, the system should undergo a Wigner transition

Model

How to change r_S?

$$r_S \propto \frac{1}{N}\frac{L}{a_B}$$

- Changing the number of particles:
  Would change Fermi-level and hence the current (no interaction effect)
- Changing the system size:
  Comparison of x-dependent quantities (e.g. density, ELF etc.) between systems of different sizes difficult
- Solution: Change Bohr radius by changing the effective electron mass [a]

[a] Markus Hofmann, PhD thesis, Universität Erlangen-Nürnberg (2005)

Model

Directly change $\frac{\langle V_C \rangle}{\langle T \rangle}$ by changing the effective electron mass:

- replace "true" effective electron mass m_0^* by a fictitious one m^* in the kinetic energy operator
- renormalize the impurity potential $V_{\mathrm{imp}} \longrightarrow V_{\mathrm{imp}} \frac{m_0^*}{m^*}$
- calculate all observables (especially current density) using the true effective electron mass m_0^*

$\Rightarrow$ persistent current of a system of non-interacting electrons independent of r_S

Density Functional Theory

How to solve the interacting problem with impurity?

Density Functional Theory

- One-to-one correspondence between external potential and electronic density
- All observables are functionals of the density
- How to use this: Construct a non-interacting system in some effective potential that gives the same density

Current Density Functional Theory

DFT with gauge field

- Ordinary DFT: basic variable $n(\vec{r})$
  - Kohn-Sham orbitals give (in principle) exact density of the interacting system
  - Not guaranteed that current density of the KS-System coincides with the current density of the interacting system
- Current Density Functional Theory: basic variable $n(\vec{r})$ and $\vec{j}_{\mathrm{p}}(\vec{r})$
  - In addition to $v_{\mathrm{xc}} = \frac{\delta E_{\mathrm{xc}}}{\delta n}$ an xc vector potential $\vec{A}_{\mathrm{xc}} = \frac{\delta E_{\mathrm{xc}}}{\delta \vec{j}_{\mathrm{p}}}$ enters the KS-equation
  - KS-orbitals yield exact density and current density

Current Density Functional Theory

Gauge invariance of the xc-functional

- Total energy has to be gauge invariant, but paramagnetic current density $\vec{j}_\mathrm{p}$ is not:

$$\vec{j}'_\mathrm{p}(\vec{r}) = \vec{j}_\mathrm{p}(\vec{r}) + \frac{e}{m} n(\vec{r}) \nabla \Lambda(\vec{r})$$

- E_H and E_ext are gauge invariant
- Gauge transformation for the non-interacting functional:

$$T_\mathrm{S}[n, \vec{j}'_\mathrm{p}] = T_\mathrm{S}[n, \vec{j}_\mathrm{p}] + e \int d\vec{r}\, \vec{j}_\mathrm{p}(\vec{r}) \nabla \Lambda(\vec{r}) + \frac{e^2}{2m} \int d\vec{r}\, n(\vec{r}) \left|\nabla \Lambda(\vec{r})\right|^2$$

- Same transformation holds for the interacting functional, hence E_xc has to be gauge invariant
- E_xc depends on $\vec{v} = \nabla \times \frac{\vec{j}_\mathrm{p}}{n}$ rather than on $\vec{j}_\mathrm{p}$ directly

Current Density Functional Theory

Local approximation

- Local approximation of the xc-functional in the variable $\nabla \times \frac{\vec{j}_\mathrm{p}}{n}$ leads to xc-vector potential [a]

$$A_\mathrm{xc} \propto \frac{1}{n} \nabla \times \left(\nabla \times \frac{\vec{j}_\mathrm{p}}{n} \right)$$

- This vanishes for strictly 1D systems
- Physical reason:
  - xc-vector potential describes distortion of the wave function in the presence of currents
  - in strictly 1D systems any distortion is purely longitudinal, only changing the density

[a] G.Vignale and M.Rasolt, Phys.Rev.B **37**, 10685 (1988)

Kohn-Sham equations

Kohn-Sham system

A non-interacting system in some effective potential that produces the same density

$$\left[\frac{1}{2m^*}\left(-i\hbar\frac{d}{dx}-eA\right)^2+v_{\mathrm{imp}}+v_{\mathrm{H}}+v_{\mathrm{xc}}\right]\varphi_i=\varepsilon_i\varphi_i$$

with

- electrostatic Hartree potential v_{H}
- exchange-correlation potential v_{xc} contains all many-body quantum effects

Approximate xc-functional

Local density approximation

- Idea: treat the inhomogeneous system locally as a homogeneous one
- xc-energy of the inhomogeneous system is a sum (integral) of all the contributions from different points of the system:

$$E_{\mathrm{xc}}[n(\vec{r})] = \int d\vec{r}\, n(\vec{r}) e_{\mathrm{xc}}(n(\vec{r}))$$

Optimized Effective Potential

- Minimize the xc-energy not with respect to the density but with respect to the KS-orbitals
- OEP potential is an explicit functional of the KS-orbitals
- Correct $\frac{1}{r}$ dependency of the xc-potential for $r \longrightarrow \infty$

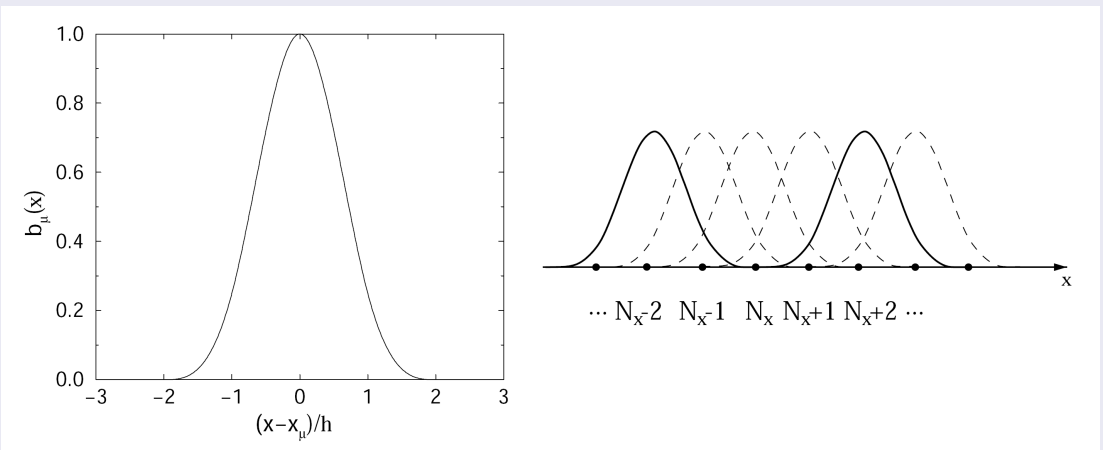
Representation of the wave functions

Spline represention

- Expansion in a set of basis functions:

$$\varphi_i(x) = \sum_{\mu} a_{\mu}^{(i)} b_{\mu}(x)$$

- Chose a localized spline basis [a]



[a] Markus Hofmann, PhD thesis, Universität Erlangen-Nürnberg (2005)

Kohn-Sham equation in the spline basis

Generalized eigenvalue problem

- Matrix representation of the KS-Hamiltonian

$$H^{\mathrm{KS}}_{\mu,\nu} = \langle b_\mu | \hat{H}_{\mathrm{KS}} | b_\nu \rangle = \int_{-\infty}^{\infty} dx\, b_\mu(x) \hat{H}_{\mathrm{KS}}\, b_\nu(x)$$

- Non-zero overlap of different basis functions leads to overlap matrix

$$S_{\mu,\nu} = \int_{-\infty}^{\infty} dx\, b_\mu(x) b_\nu(x)$$

- Matrix representation of the Kohn-Sham equation

$$\sum_\nu H^{\mathrm{KS}}_{\mu,\nu} a^{(i)}_\nu = \varepsilon_i \sum_\nu S_{\mu,\nu} a^{(i)}_\nu$$

Self-consistent solution of the KS-equation

Single iteration cycle

- Decompostion of the overlap matrix $\hat{S} = \hat{L}\hat{L}^{\mathrm{T}}$ leads to a standard eigenvalue problem

$$\left[\hat{L}^{-1}\hat{H}_{\mathrm{KS}}(\hat{L}^{\mathrm{T}})^{-1}\right]\left(L^{\mathrm{T}}\vec{a}^{(i)}\right) = \varepsilon_i\left(\hat{L}^{\mathrm{T}}\vec{a}^{(i)}\right)$$

- Matrix $\left[\hat{L}^{-1}\hat{H}_{\mathrm{KS}}(\hat{L}^{\mathrm{T}})^{-1}\right]$ is numerically diagonalized
- Resulting eigenvector $\left(L^{\mathrm{T}}\vec{a}^{(i)}\right)$ is transformed back to $\vec{a}^{(i)}$
- $\vec{a}^{(i)}$ represents the eigenstates of the Hamiltonian $\hat{H}_{\mathrm{KS}}$

Self-consistent solution of the KS-equation

Self-consistent scheme

- Start with a non-interacting system: $v_{\mathrm{H}} = 0$ and $v_{\mathrm{xc}} = 0$
- Solve KS-equations $\Rightarrow$ density $n(x)$
- Calculate Hartree- and xc-potential from the density
- Solve KS-equation with new v_{H} and v_{xc}

Convergence criterion:

$$\max_i \left| \varepsilon_i^{(n)} - \varepsilon_i^{(n-1)} \right| < 10^{-10}\mathrm{meV}$$

Persistent current

Calculation of the current density

- Paramagnetic current density of a state $|\varphi_i\rangle$

$$j_{\mathrm{p}}^{(i)}(x) = -\frac{i\hbar}{2m_0^*}\left(\varphi_i^*(x)\frac{d}{dx}\varphi_i(x) - \varphi_i(x)\frac{d}{dx}\varphi_i^*(x)\right)$$

- Diamagnetic current density

$$j_{\mathrm{d}}(x) = -\frac{\hbar}{m_0^*}\frac{2\pi}{L}\frac{\Phi}{\Phi_0}n(x)$$

- Total current density

$$j(x) = \sum_{i=1}^{N} j_{\mathrm{p}}^{(i)}(x) + j_{\mathrm{d}}(x)$$

Persistent current

What has been done

Persistent current has been calculated at 0.3 of the flux quantum for

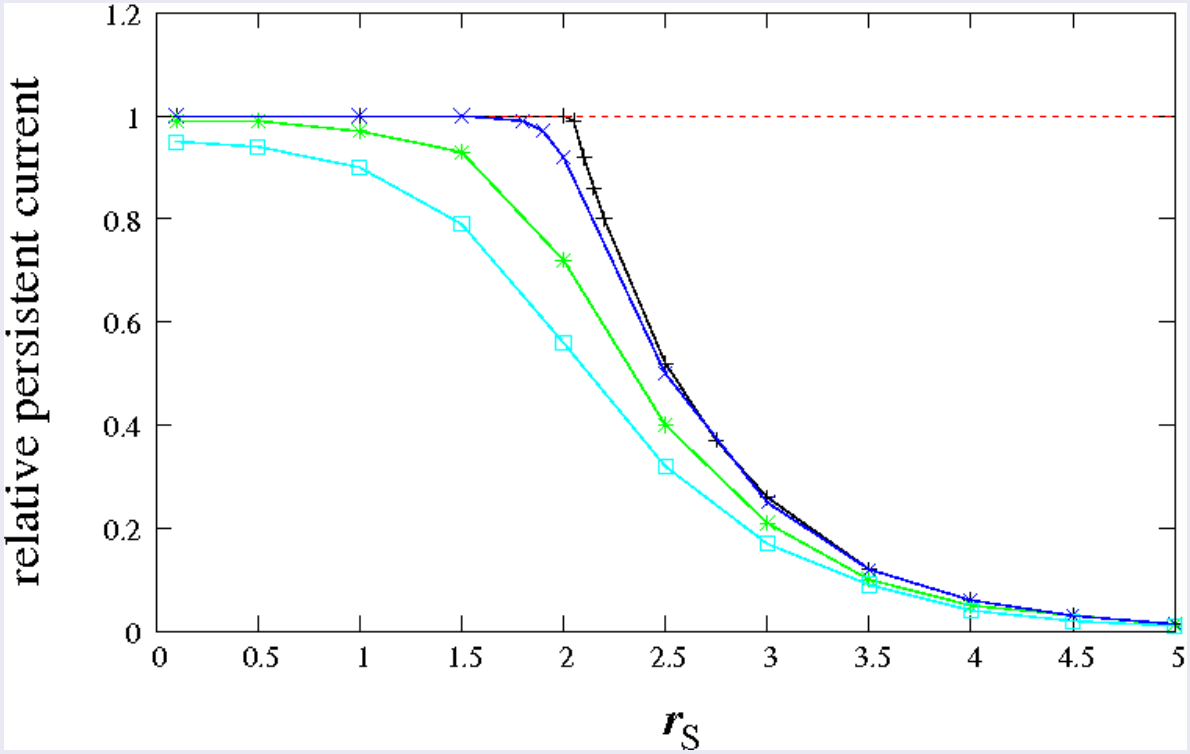
- several values of r_S
- different impurity potential strengths

Computational parameters

- System size $L = 200$nm
- 540 basis functions
- Typically between 100 (far from the transition point) and 10000 (close to the transition point) iterations for full convergence required

Persistent current

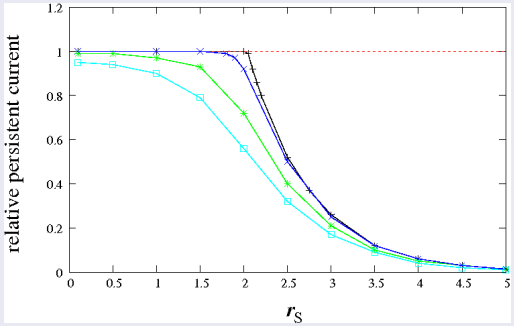
Persistent current as a function of r_S



Colors indicate (unrenormalized) pinning potential strength: black $V_0 = 0.001$meV, blue $V_0 = 1.0$meV, green $V_0 = 5.0$meV, light blue $V_0 = 10.0$meV; red dashed line: noninteracting system with $V_0 = 0.001$meV

Persistent current as a function of r_S

Very weak impurity potential



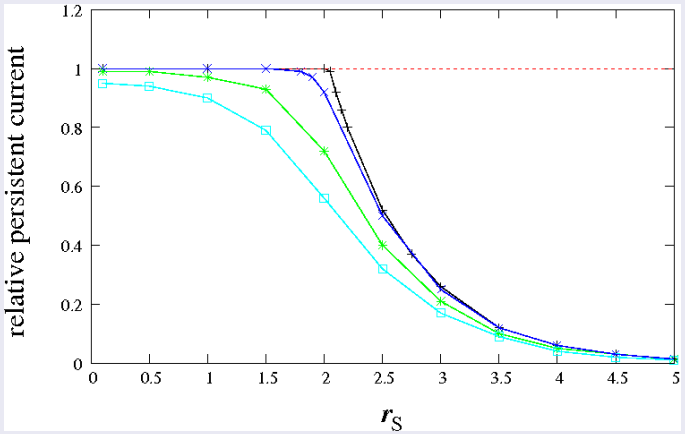
Very weak impurity (on the scale of the internal energy of the crystal $\approx 2 - 5$meV):

- $r_S < r_S^c$: persistent current independent of r_S
- $r_S > r_S^c$: persistent current decays exponentially with increasing r_S
- Interpretation: Wigner crystal transition at $r_S^c \approx 2.05$ (2D: $r_S^c \approx 37 \pm 5$)[a]

[a] B.Tanatar and C.M.Ceperly, Phys.Rev.B **39**, 5005 (1989)

Persistent current as a function of r_S

Non-vanishing impurity

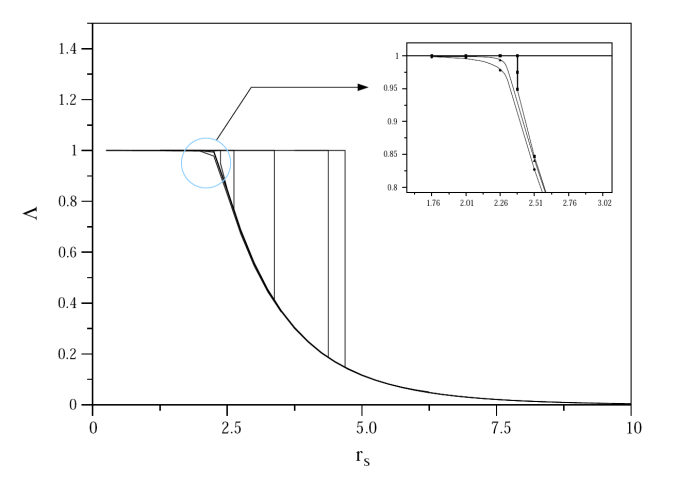


For stronger impurity:

- Transition shifted to smaller r_S and smoothed
- Even for very small r_S no electron-gas like behaviour:
  No range where the persistent current is independent of r_S

Total energy curvature as a localization criterion

Relative curvature of the ground state energy as a function of r_S [a]



- Localization for $r_S > r_S^c$
- Critical value of r_S strongly depends on disorder
- Transition point consistent with results from calculation of the persistent current

[a] Markus Hofmann, PhD thesis, Universität Erlangen-Nürnberg (2005)

Summary and Outlook

What has been done

- Electron-electron interactions may drastically change the persistent current in a one-dimensional ring
- Interpretation: Formation and pinning of a Wigner crystal phase at $r_S \approx 2.05$
- Form of the transition depends on the strength of the pinning potential:
  - Very weak pinning potential leads to a sharp transition
  - Stronger (but still weak) pinning potentials lead to a smooth transition

Still to do

- Study the dependence of the Wigner crystal transition on the shape and width of the pinning potential
- Extension to two-dimensional rings