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

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Experimental situation

- Effectively one-dimensional system can be realized experimentally
- Number of electrons can be controlled 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
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 → sensitive to the boundary conditions → large value for the curvature
  - Localized system → insensitive to the boundary conditions → 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-interacting particles concerning the persistent 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\(^\text{a}\)

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

Model

One-dimensional quantum ring

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

Hamiltonian

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

with

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

One-dimensional Wigner-Seitz radius $r_S$

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

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

with the Bohr radius

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

In GaAs ($\epsilon = 12.5$, $m^*_0 = 0.0665m_e$): $a_B = 9.95 \cdot 10^{-9} m$

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

\(^a\text{Markus Hofmann, PhD thesis, Universität Erlangen-Nürnberg (2005)}\)
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 $V_{\text{imp}} \rightarrow V_{\text{imp}} \frac{m_0^*}{m^*}$
- 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 $\vec{j}_p(\vec{r})$
  - In addition to $\nu_{xc} = \frac{\delta E_{xc}}{\delta n}$ an xc vector potential $\vec{A}_{xc} = \frac{\delta E_{xc}}{\delta \vec{j}_p}$ 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 $\vec{j}_p$ is not:

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

- $E_H$ and $E_{\text{ext}}$ are gauge invariant

- Gauge transformation for the non-interacting functional:

$$T_S[n, \vec{j}'_p] = T_S[n, \vec{j}_p] + e \int d\vec{r} \vec{j}_p(\vec{r}) \nabla \Lambda(\vec{r}) + \frac{e^2}{2m} \int d\vec{r} n(\vec{r}) |\nabla \Lambda(\vec{r})|^2$$

- Same transformation holds for the interacting functional, hence $E_{\text{xc}}$ has to be gauge invariant

- $E_{\text{xc}}$ depends on $\vec{\nu} = \nabla \times \frac{\vec{j}_p}{n}$ rather than on $\vec{j}_p$ directly
Local approximation

- Local approximation of the xc-functional in the variable $\nabla \times \frac{\vec{j}_p}{n}$ leads to xc-vector potential $^a$

\[
A_{xc} \propto \frac{1}{n} \nabla \times \left( \nabla \times \frac{\vec{j}_p}{n} \right)
\]

- 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

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Kohn-Sham equations

Kohn-Sham system

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

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

with

- electrostatic Hartree potential $v_H$
- exchange-correlation potential $v_{\text{xc}}$ 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:

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

#### 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 \( r \to \infty \).
Representation of the wave functions

Spline representation

- Expansion in a set of basis functions:

\[ \varphi_i(x) = \sum_{\mu} a^{(i)}_\mu b_\mu(x) \]

- Chose a localized spline basis \(^a\)

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\(^a\)Markus Hofmann, PhD thesis, Universität Erlangen-Nürnberg (2005)
Generalized eigenvalue problem

- Matrix representation of the KS-Hamiltonian

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

- 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

\[ \sum_{\nu} H_{\mu,\nu}^{KS} a_\nu^{(i)} = \varepsilon_i \sum_{\nu} S_{\mu,\nu} a_\nu^{(i)} \]
Single iteration cycle

- Decomposition of the overlap matrix $\hat{S} = \hat{L}\hat{L}^T$ leads to a standard eigenvalue problem
  \[
  \left[ \hat{L}^{-1}\hat{H}_{\text{KS}}(\hat{L}^T)^{-1} \right] \left( L^T\vec{a}^{(i)} \right) = \varepsilon_i \left( \hat{L}^T\vec{a}^{(i)} \right)
  \]
- Matrix $\left[ \hat{L}^{-1}\hat{H}_{\text{KS}}(\hat{L}^T)^{-1} \right]$ is numerically diagonalized
- Resulting eigenvector $(L^T\vec{a}^{(i)})$ is transformed back to $\vec{a}^{(i)}$
- $\vec{a}^{(i)}$ represents the eigenstates of the Hamiltonian $\hat{H}_{\text{KS}}$
Self-consistent solution of the KS-equation

Self-consistent scheme

- Start with a non-interacting system: \( v_H = 0 \) and \( v_{xc} = 0 \)
- 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:

\[
\max_i \left| \varepsilon_i^{(n)} - \varepsilon_i^{(n-1)} \right| < 10^{-10} \text{meV}
\]
Persistent current

Calculation of the current density

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

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

- Diamagnetic current density

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

- Total current density

$$ j(x) = \sum_{i=1}^{N} j_p^{(i)}(x) + j_d(x) $$
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 $L = 200\text{nm}$
- 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 as a function of $r_S$

Colors indicate (unrenormalized) pinning potential strength: black $V_0 = 0.001\text{meV}$, blue $V_0 = 1.0\text{meV}$, green $V_0 = 5.0\text{meV}$, light blue $V_0 = 10.0\text{meV}$; red dashed line: noninteracting system with $V_0 = 0.001\text{meV}$.
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 $\approx 2 - 5\text{meV}$):

- $r_S < r_S^c$: 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: $r_S^c \approx 37 \pm 5)^a$

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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 $r_S$

- 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

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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.