From Fabry-Perot oscillations to Coulomb blockade in a quantum wire

Varvara Petrova

P3TMA computer project supervised by Adeline Crépieux
Aix-Marseille University

February 24, 2017

Outline

- Introduction
- Results of Dyson approach technique
- Numerical methods and optimization
- Results
- Conclusion

Introduction

We consider an infinite one-dimensional interacting quantum wire (QW) with two impurities of arbitrary potential strength at positions $x_{1,2} = \pm L/2$.

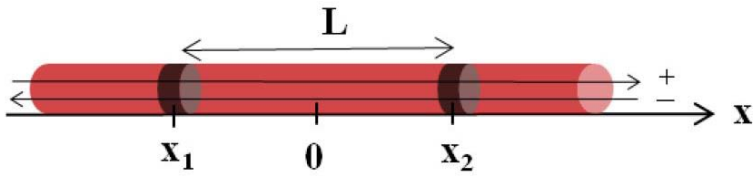


FIG. 1: The right (+) and left (−) chiralities are denoted by right and left arrows.

- Let $\rho(x, \omega)$ be the local density of states of the system.
  How does the impurity potential strength changes its 2D-profile?
  What is the interplay between interactions and impurities?

- The aim of the project is to take the results of Dyson approach technique and to compute $\rho(x, \omega)$ using *Mathematica*.

- Characteristic scales:
  - length: a, the small-distance cut-off of the Tomonaga-Luttinger theory;
  - energy: $\hbar\omega_c$, where $\omega_c = v_F/a$ is a cut-off frequency, v_F being the Fermi velocity.

Results of Dyson approach technique

Dimensionless equations to be solved

- Local density of states (LDOS): $\rho(x,\omega) = -\frac{1}{\pi}\sum_{r,r'} \mathrm{Im}\left\{G^R_{r,r'}(x,x;\omega)\right\}$
- Retarded Green's function:

$$G^R_{r,r'}(x,x';\omega) = g^R_r(x,x';\omega)\delta_{r,r'} + \sum_{i=1,2} g^R_r(x,x_i;\omega)\left[\Gamma^B_i G^R_{-r,r'}(x_i,x';\omega) + \Gamma^F_i G^R_{r,r'}(x_i,x';\omega)\right] \quad (1)$$

Expressions of $G^R_{r,r}(x_i,x';\omega)$ and $G^R_{-r,r}(x_i,x';\omega)$ can be extracted from (1) by solving a linear set of equations.

$$g^R_r(x,x';\omega) \overset{x\neq x'}{=} \frac{-e^{irk_F(x-x')}K^2\omega_+}{2\sqrt{\pi}\Gamma(1+\gamma)}\left(\frac{2i|x-x'|}{K\omega_+}\right)^{\frac{1}{2}-\gamma} \times\left[\mathbf{K}_{\gamma-\frac{1}{2}}\left(-iK|x-x'|\omega_+\right) - \mathrm{sgn}\left(r(x-x')\right)\mathbf{K}_{\gamma+\frac{1}{2}}\left(-iK|x-x'|\omega_+\right)\right]$$

$$\text{and}\quad g^R_r(x,x;\omega) \approx -\frac{\Gamma(\frac{1}{2}-\gamma)K^2\omega_+}{4\sqrt{\pi}\Gamma(1+\gamma)}\left(\frac{K\omega_+}{2i}\right)^{2\gamma-1}$$

- Γ and $\mathbf{K}$ are the Gamma and modified Bessel functions; K controls the interaction strength ($K=1$ no interaction, $0<K<1$ repulsive (Coulomb) interaction); $\gamma := (K+K^{-1}-2)/4$; $\omega_+ := \omega + i\epsilon$ ($\epsilon>0$). $\Gamma^{B,F}_{1,2}$ correspond to backward and forward impurity potential strengths. To simplify, we shall take $\Gamma^B_{1,2} = \Gamma^F_{1,2} \equiv \Gamma$.

Numerical methods

- **Method 1** (naive approach): directly input the formulas using the analytical expressions of $G^R_{r,r}(x_i, x'; \omega)$ and $G^R_{-r,r}(x_i, x'; \omega)$.
  $\rightarrow$ Not efficient. The execution time t_{exec} per 2D graph is ~ 27 min.
- **Method 2**: numerically compute $G^R_{r,r}(x_i, x'; \omega)$ and $G^R_{-r,r}(x_i, x'; \omega)$ by solving a system of linear equations, $MX = B$, where:

$$M = \begin{pmatrix} 1 - \Gamma g^R_+(x_1, x_1; \omega) & -\Gamma g^R_+(x_1, x_1; \omega) & -\Gamma g^R_+(x_1, x_2; \omega) & -\Gamma g^R_+(x_1, x_2; \omega) \\ -\Gamma g^R_-(x_1, x_1; \omega) & 1 - \Gamma g^R_-(x_1, x_1; \omega) & -\Gamma g^R_-(x_1, x_2; \omega) & -\Gamma g^R_-(x_1, x_2; \omega) \\ -\Gamma g^R_+(x_2, x_1; \omega) & -\Gamma g^R_+(x_2, x_1; \omega) & 1 - \Gamma g^R_+(x_2, x_2; \omega) & -\Gamma g^R_+(x_2, x_2; \omega) \\ -\Gamma g^R_-(x_2, x_1; \omega) & -\Gamma g^R_-(x_2, x_1; \omega) & -\Gamma g^R_-(x_2, x_2; \omega) & 1 - \Gamma g^R_-(x_2, x_2; \omega) \end{pmatrix} \otimes \mathbb{1}_2$$

$\mathbb{1}_2$ is the two-dimensional identity matrix; X and B are 8-component column-vectors:

$$X(x'; \omega) = {}^t\Big(G^R_{+,+}(x_1, x'; \omega), G^R_{+,-}(x_1, x'; \omega), G^R_{-,+}(x_1, x'; \omega), G^R_{-,-}(x_1, x'; \omega), G^R_{+,+}(x_2, x'; \omega), G^R_{+,-}(x_2, x'; \omega), G^R_{-,+}(x_2, x'; \omega), G^R_{-,-}(x_2, x'; \omega) \Big),$$

$$B(x', \omega) = {}^t\left(g^R_+(x_1, x'; \omega), 0, 0, g^R_-(x_1, x'; \omega), g^R_+(x_2, x'; \omega), 0, 0, g^R_-(x_2, x'; \omega) \right).$$

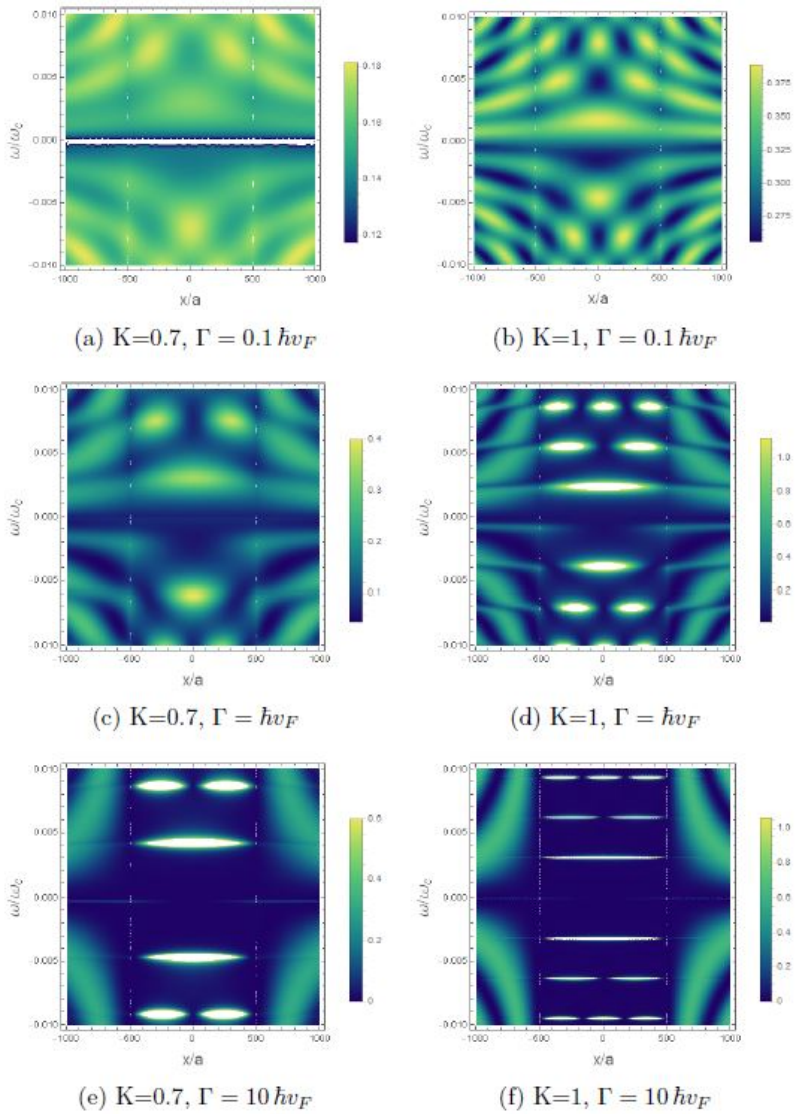
  - **Option 1**: use `LinearSolve[ ]` ($t_{exec} \sim 7$ min).
  - **Option 2**: diagonalize M first by means of `Eigenvalues[ ]` and `Eigenvectors[ ]` or `Eigensystem[ ]`.

Optimization

- Choose option 2.
- Get rid of the "`function[arguments][[index]]`" syntax using `Module[]` in the body of the function ρ`[x,`ω`]`.
- Particular attention to `PlotPoints` option in `DensityPlot[ ]` function: increase the number of samples used.
- With these improvements, $t_{exec} \sim 3$ min!

Results

- At first we take $k_F = 0$ and plot $\rho[\mathtt{x},\omega]$ in the region $[-L, L] \times [-0.01\omega_c, 0.01\omega_c]$ with $L = 1000a$.
- Convergence for $\epsilon < 10^{-5}$. Results obtained with $\epsilon = 10^{-6}$ and `PlotPoints` $\rightarrow$ 100 are in agreement with the expected LDOS profiles.
- For small-impurity potentials ($\Gamma \lesssim 0.1\,\hbar v_F$), the LDOS of the non interacting QW is odd in energy.
- In the intermediate impurity regime ($\Gamma \sim \hbar v_F$), in both cases the LDOS profile is neither odd, nor even whilst it becomes even for strong-impurity potentials.



(a) K=0.7, $\Gamma = 0.1\,\hbar v_F$ (b) K=1, $\Gamma = 0.1\,\hbar v_F$

(c) K=0.7, $\Gamma = \hbar v_F$ (d) K=1, $\Gamma = \hbar v_F$

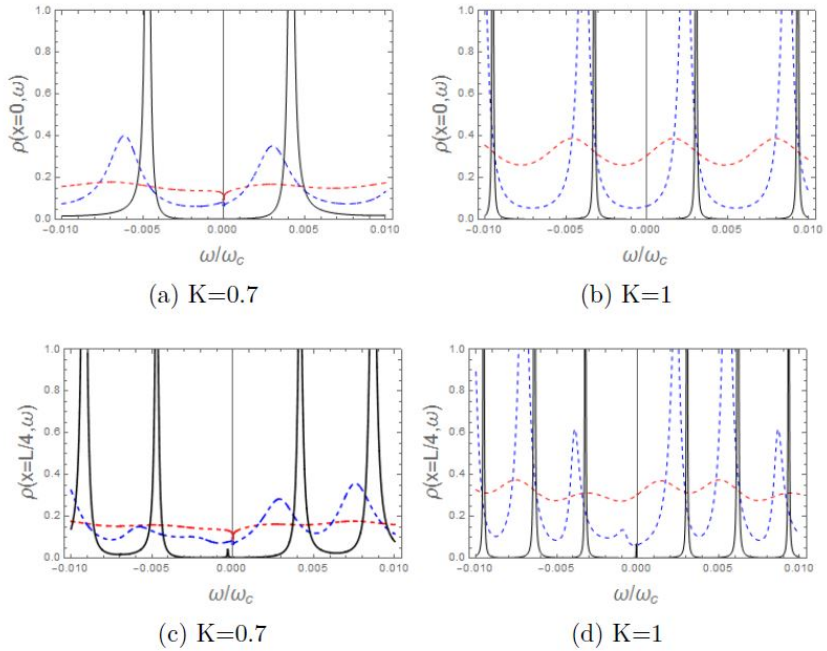
(e) K=0.7, $\Gamma = 10\,\hbar v_F$ (f) K=1, $\Gamma = 10\,\hbar v_F$

FIG. 2: LDOS in the presence of Coulomb interactions ($K = 0.7$) and for a non interacting wire ($K = 1$) as a function of position and energy.

Results

- The presence of impurities reduce the amplitude of density peaks. In case $\Gamma \geq \hbar v_F$, the weaker the interaction is ($K \to 1$), the thinner, wider, intense and frequently spaced they are.
- In the regime $\Gamma \sim 10\,\hbar v_F$, the central part of the wire becomes quasi-isolated and corresponding energy levels discrete (Coulomb-blockade).
- At fixed $\Gamma \geq \hbar v_F$, energy levels spacing s reduces as $K \to 1$ in agreement with the theory of the finite size wire of length L: $s \sim \pi v/L$ with $v = v_F/K$.

Density of states as a function of energy



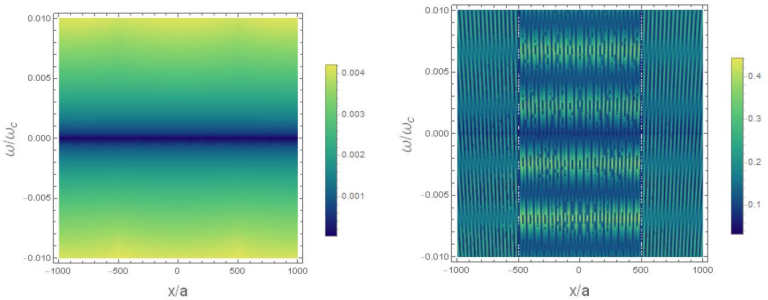
(a) K=0.7 (b) K=1

(c) K=0.7 (d) K=1

FIG. 3: LDOS in the presence of Coulomb interactions ($K = 0.7$) and for a non interacting wire ($K = 1$) as a function of energy at two different positions, $x = 0$ (upper graphs) and $x = L/4$ (bottom graphs), for $\Gamma = 0.1\,\hbar v_F$ (red dashed lines), $\Gamma = \hbar v_F$ (blue dashed lines) and $\Gamma = 10\,\hbar v_F$ (black solid lines).

Results

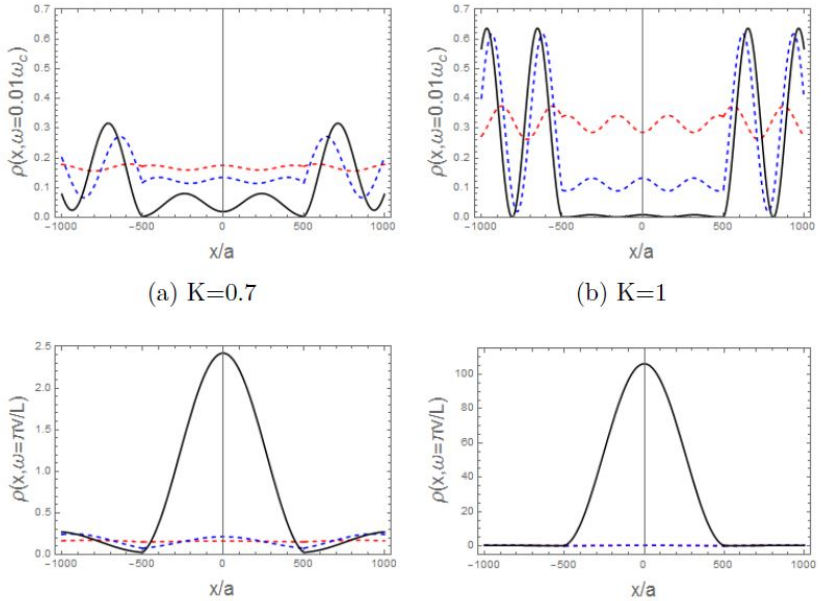
- The presence of impurities reduce the amplitude of density peaks. In case $\Gamma \geq \hbar v_F$, the weaker the interaction is ($K \to 1$), the thinner, wider, intense (and frequently spaced) they are.
- LDOS is zero on the impurities sites.
- LDOS peaks disappear completely for $K \leq 0.4$ and in the case $k_F \neq 0$, LDOS exhibits a strong oscillatory behaviour.



(a) $K = 0.35\ \Gamma = 1\,\hbar v_F\ k_F = 0$ (b) $K = 0.7\ \Gamma = 1\,\hbar v_F\ k_F = 0.1$

FIG. 5: Special cases

Density of states as a function of position



(a) K=0.7 (b) K=1

(c) K=0.7 (d) K=1

FIG. 4: LDOS in the presence of Coulomb interactions ($K = 0.7$) and for a non interacting wire ($K = 1$) as a function of position for two different frequences, $\omega = 0,01\omega_c$ (upper graphs) and $\omega \approx \pi v/L$ (bottom graphs), for $\Gamma = 0.1\,\hbar v_F$ (red dashed lines), $\Gamma = \hbar v_F$ (blue dashed lines) and $\Gamma = 10\,\hbar v_F$ (black solid lines).

Conclusion and perspectives

- We have calculated and drawn the density of states for an interacting quantum wire in presence of two impurities of equal potential strength.
- We explored different methods of solving a system of linear equations. `Eigensystem[ ]` function is the most efficient in terms of the execution time.
- The code was optimized by means of `Module[ ]` function. The importance of `PlotPoints` and `MaxRecursion` has also been noticed.
- We observed that the main effect of interactions is to reduce the amplitude of the (Fabry-Perot) oscillations in the weak impurity regime and the Coulomb-blockade peaks in the strong-impurity regime.
- More quantitative analysis of the evolution of LDOS peaks amplitude and spacing with the interaction strength K need to be performed.
  $\rightarrow$ systematic calculations based on `FindMaximum[ ]`.