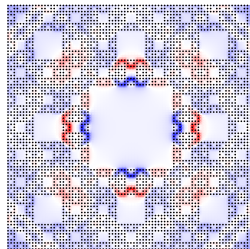
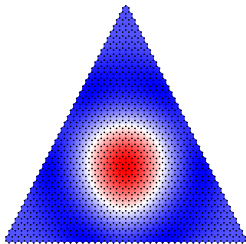


# Plasmonic Properties of QM 2D Fractals.

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TCM



# Stained Glass



# Plasmons

## Definition (Plasmon)

Quantum of plasma oscillation (*think quasiparticle*).

## Definition (Plasma Oscillation)

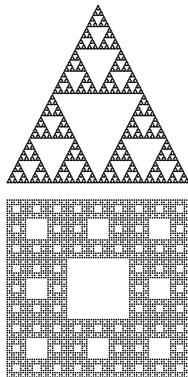
Longitudinal wave of electron charge-density.

# Fractals

- Features: nowhere differentiable, have fractal dimensions, self-similar, etc.
- Ramification: minimum number of links that one needs to remove to separate a macroscopic part of infinite fractal.

*Finite ramification:* **Solved analytically**  
by L.P. Kadanoff (1982).

*Infinite ramification:* **Unsolvable analytically** (?). Numerical calculations exist (*done at Radboud*), but not of plasmonic properties.



# Tight Binding

- atomic basis  $\{|a\rangle\}$
- Hamiltonian of the system is

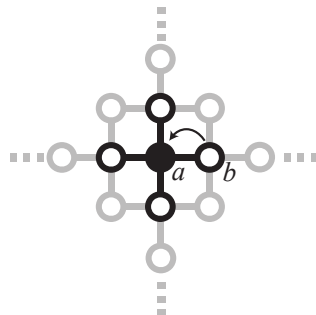
$$\hat{\mathcal{H}} = -t \sum_{\langle a,b \rangle} (\hat{c}_a^\dagger \hat{c}_b + \text{h.c.}) ,$$

$\hat{c}_a^\dagger$  and  $\hat{c}_a$  are creation and annihilation operators,  $t$  is the hopping value.

- Hopping:

$$\underbrace{\hat{c}_a^\dagger \hat{c}_b}_{\text{"take" from } b} |\psi\rangle$$

"move" to  $a$



# System

- Electron system is described (in one-particle approximation) by
  - eigenenergies  $\{E_i\}$  and
  - eigenstates  $\{|i\rangle\}$ .
- Grand-canonical ensemble, i.e. temperature  $T$  and chemical potential  $\mu$  are fixed.
- Occupational numbers are given by the Fermi-Dirac distribution.

# Problem

- All plasmonic properties are obtained from the **dielectric function**  $\hat{\epsilon}$ .  
⇒ Goal: **calculate**  $\hat{\epsilon}$ .
- There exist good methods for calculation of the dielectric function in **momentum space**, i.e. they rely on translational symmetry of the system.
- But in fractals, there is **no translational symmetry**!
- Calculations have to be done in **real space**.  
⇒ **New method**.

# Dielectric Function in Real Space

Within the Random Phase Approximation (RPA) we obtain:

$$\langle \mathbf{r} | \hat{V}_{\text{ext}}(\omega) | \mathbf{r} \rangle = \int d^3 r' \langle \mathbf{r} | \hat{\epsilon}(\omega) | \mathbf{r}' \rangle \langle \mathbf{r}' | \hat{V} | \mathbf{r}' \rangle, \text{ where}$$

$$\begin{aligned} \langle \mathbf{r} | \hat{\epsilon}(\omega) | \mathbf{r}' \rangle = \langle \mathbf{r} | \mathbf{r}' \rangle - \lim_{\eta \rightarrow 0+} \sum_{i,j} \frac{n_i - n_j}{E_i - E_j - \hbar(\omega + i\eta)} \int d^3 r'' \frac{e^2}{\|\mathbf{r} - \mathbf{r}''\|} \\ \times \langle j | \mathbf{r}'' \rangle \langle \mathbf{r}'' | i \rangle \langle i | \mathbf{r}' \rangle \langle \mathbf{r}' | j \rangle. \end{aligned}$$



# Algorithm

Calculating  $\hat{\epsilon}$  for a single  $\omega$  is an  $\mathcal{O}(N^4)$  problem, where  $N$  is the number of particles.

- Hack: rewrite everything in terms of **matrix operations** and use BLAS (*Basic Linear Algebra Subroutines*).
- Use a **supercomputer** for calculations.
- Hack: use **symmetries** of the system.

# Code

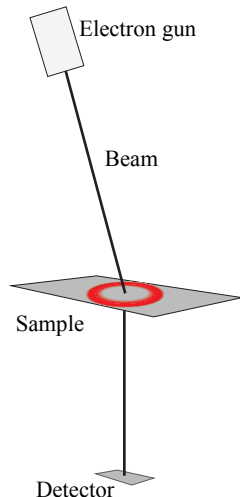
- Written C++ package to calculate  $\hat{\varepsilon}$  for a **general** system described by TB.
- **$\approx 8.5$  thousands** lines of code (*excluding* data analysis scripts).
- $\approx 400000$  computational hours spent, that is  **$\approx 45$  years of calculations.**

# Electron Energy Loss Spectroscopy (EELS)

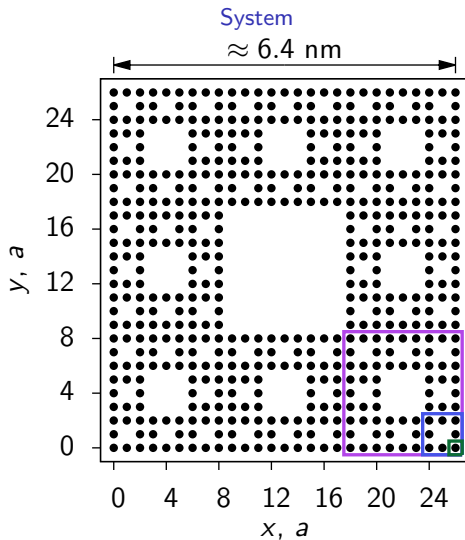
- Shoot electrons on the sample.
  - Electron beam with a well-defined four-momentum  $p^\mu$ .
  - Inelastic scattering results in **energy loss  $E = \hbar\omega$**  and **momentum transfer  $\hbar\mathbf{q}$** .
- Look at (usually) transmitted electrons.

double-differential  
cross section

$$\overbrace{\frac{d^2\sigma}{d\Omega dE}} \propto \underbrace{-\text{Im} \left[ \frac{1}{\langle \mathbf{q} | \hat{\epsilon}(\omega) | \mathbf{q} \rangle} \right]}_{\text{loss function}}.$$

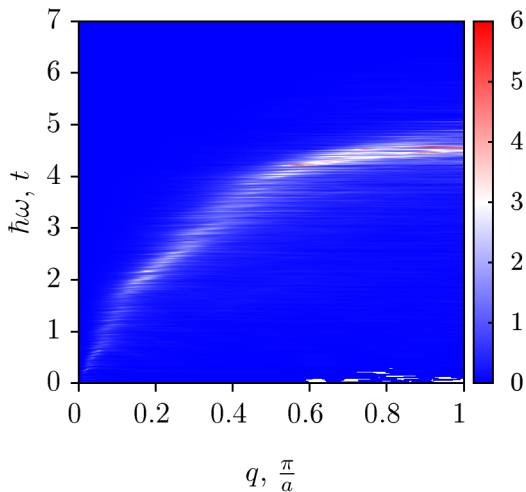


## Third Iteration Sierpinski Carpet



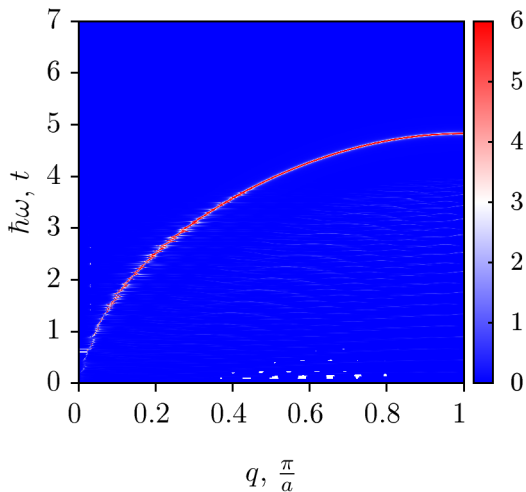
# Third Iteration Sierpinski Carpet

## Results



# Square Lattice

## Results



## Summary

- It *is* possible to do calculations of  $\hat{\epsilon}$  in real space.
- There *are* well defined plasmons in Sierpinski carpets, which is *unexpected* for a system without translational invariance.
- The created package can be *reused* to study plasmonic properties of other systems.

# Outlook

- Publish the results, i.e. write a paper.
- Look at *other* systems with no translational symmetry.



Any questions?

## Simple example of plasma oscillation

- Free electron gas with positively charged atom cores in the background.
- Oscillating electric field  $\mathbf{E}(t) = \mathbf{E}_0 \exp(-i\omega t)$ .
- Equation of motion:

$$\ddot{\mathbf{x}} + \gamma \dot{\mathbf{x}} = -\frac{e}{m} \mathbf{E}(t) .$$

- Displaced electrons generate a polarization  $\mathbf{P} = -Nex$  ( $N$  is the electron density).
- From  $\epsilon_0 \mathbf{E} + \mathbf{P} = \epsilon_0 \epsilon(\omega) \mathbf{E}$  we get  $\epsilon(\omega)$ .
- In high frequency limit  $\epsilon(\omega) \approx 1 - \frac{\omega_p^2}{\omega^2}$ ,  
 $\omega_p$  — **plasma frequency**.
- If  $\omega = \omega_p$ , we get longitudinal oscillation of electron-charge density.

## Random Phase Approximation

- Perturbation of the form

$$\hat{V} e^{-i(\omega+i\eta)t}, \text{ with } \eta \rightarrow +0.$$

( $\hat{V}$  is diagonal in  $\mathbf{r}$ -basis, i.e.  $\langle \mathbf{r} | \hat{V} | \mathbf{r}' \rangle = V(\mathbf{r}) \delta^3(\mathbf{r} - \mathbf{r}')$ )

- Results in an induced charge density variation  $\delta \hat{N}(t)$
- Self-consistency equation

$$\langle \mathbf{r} | \hat{V}_{\text{tot}}(t) | \mathbf{r} \rangle = \langle \mathbf{r} | \hat{V}_{\text{ext}}(t) | \mathbf{r} \rangle + \int d^3 r' \langle \mathbf{r} | \hat{V}_{\text{Coulomb}} | \mathbf{r}' \rangle \langle \mathbf{r}' | \delta \hat{N}(t) | \mathbf{r}' \rangle.$$