Diploma Thesis

“Analysis of Dynamics in Phase Space by means of the Zeros of the Husimi Function”

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solid-state-physics: models for metals and insulators?
we consider the Anderson-Model and Aubry-André-Model
Phase Space give simultaneous access to location and momentum information of conduction electrons
Husimi Function represents quantum state in phase space
How does the Husimi Function change during the metal-insulator-transition? How can these changes be described or quantified?
⇒ qualitative and quantitative description of the dynamics by means of the zeros of the Husimi Function
How can the behaviour of metals and insulators be modelled?
Can one simulate a “phase transition” between them?

⇒ different approaches: bonding model, doping, impurities, ...

here: impurities in the crystal lattice potential are considered

⇒⇒ We expect a transition from metal to insulator when the “strength” of the impurities is increased.
How to model the transition?

⇒ use a simple model:

- consider a single $e^-$ on an infinite lattice
- the $e^-$ can hop between neighboring lattice sites
- impurities are modelled as irregularities in the potential
- atomic potential not relevant
- for numerical calculations: restriction to the 1D case
Hamiltonian of the Anderson-Model (1958):

\[ \mathcal{H} = - \sum_{x = -\infty}^{\infty} \left( |x+1\rangle \langle x| + |x\rangle \langle x+1| \right) + W \sum_{x = -\infty}^{\infty} v_x |x\rangle \langle x| \]

- \( x \) denotes the position of the lattice site
- \( |x+1\rangle \langle x| \) and \( |x\rangle \langle x+1| \) are the hopping matrix entries (transition probabilities between neighboring lattice sites)
- \( |x\rangle \langle x| \) stands for the potential energy at lattice site \( x \)
- \( v_x \in [-\frac{1}{2}, \frac{1}{2}] \) denotes the relative disorder strength at \( x \) (the \( v_x \) are randomly chosen and then remain fixed)
- \( W \geq 0 \) is the global disorder strength and can be varied
Hamiltonian of the Aubry-André-Model (1980):

\[ H = - \sum_{x = -\infty}^{\infty} (|x + 1\rangle \langle x| + |x\rangle \langle x + 1|) + \lambda \sum_{x = -\infty}^{\infty} \cos(2\pi \beta x) |x\rangle \langle x| \]

- single difference to Anderson: other disorder potential
- here the potential is not random, but deterministic
- \[ \beta := \frac{\sqrt{5} - 1}{2} \] is irrational
  \[ \implies \cos(2\pi \beta x) \] is not a periodic, but quasiperiodic potential
- \( \lambda \geq 0 \) is the global disorder strength (equivalent to \( W \geq 0 \))
Comparison of the potentials:

- random potential
- quasiperiodic potential
- periodic potential
How to calculate these model systems numerically?

- only finite systems are computable: 
  \[ \sum_{x = -\infty}^{\infty} \rightarrow \sum_{x = 0}^{L-1} \]
- for this, consider a periodic ring with \( L \) lattice sites
- periodic boundary condition: \( |L\rangle := |0\rangle \)

\[ \Rightarrow \text{allowed values for the electron's position and momentum:} \]

\[ x \in [0, L) \quad x = 0, 1, \ldots, L - 1 \]

\[ k \in [-\pi, \pi) \quad k = -\pi, -\frac{L-2}{L}\pi, \ldots, \frac{L-2}{L}\pi \]

the above values of \( k \) result from

- the periodicity of \( |\psi\rangle \)
- the convention to choose \( k \) from the first Brillouin zone
for a system with $L$ lattice sites, $\mathcal{H}$ is a $L \times L$ matrix

- $\mathcal{H} \psi(x) = E \psi(x)$ is solved by diagonalization of $\mathcal{H}$
- $\mathcal{H}$ is real and symmetric $\Rightarrow$ fast routines with $O(L^3)$ available
- Aubry-André-Model: quasiperiodicity allows $\mathcal{H}$ to be decomposed into two real, symmetric and tridiagonal matrices $\Rightarrow$ especially fast solvable

upon diagonalization, $L$ eigenvalues and eigenvectors are obtained
Husimi Function

Advantage of phase space representations in physics: simultaneous information about position and momentum of objects is available (as opposed to position and momentum representation)

- **classical physics**: object’s state is well defined at arbitrary times by a point in phase space
- **quantum physics**: Heisenberg uncertainty principle $\Rightarrow$ quantum object “smeared out” in phase space

How to obtain a quantum phase space representation of a given quantum state $|\psi\rangle$?
there is no unique phase space representation in QM
several useful representations have been proposed, e.g.

**Wigner Function:**

\[
W(x, k) = \frac{1}{2\pi} \int dx' \ e^{ikx'} \ \psi^* \left( x + \frac{x'}{2} \right) \psi \left( x - \frac{x'}{2} \right)
\]

**Husimi Function:**

\[
Q(x, k) = 2 \int dx' \ dk' \ \exp \left( - \frac{(x - x')^2}{2\sigma^2} - 2\sigma^2 (k - k')^2 \right) W(x', k')
\]

- The Husimi Function can be obtained from the Wigner Function by “smearing” \( W \) with a Gauß Function.
- \( \sigma \) is the ratio of the position and momentum smears.
Properties of the Husimi Function:

- positive definite: $0 \leq Q(x, k) \leq 1$ (contrary to the Wigner Function)
- can be regarded as a probability distribution in phase space
- equivalent definition as the projection of the quantum state onto a coherent state:

**Husimi Function (alternative definition):**

$$Q(x, k) = \left| \int dx' \langle x, k | x' \rangle \langle x' | \psi \rangle \right|^2 = |\langle x, k | \psi \rangle|^2$$

with the wavefunction $\langle x | \psi \rangle = \psi(x)$ and the coherent state $|x_0, k_0\rangle$ in position representation

$$\langle x | x_0, k_0 \rangle = (2\pi \sigma^2)^{-\frac{1}{4}} \exp \left( -\frac{(x - x_0)^2}{4\sigma^2} + ik_0x \right)$$
numerically, the Husimi Function can be calculated from $\psi(x)$ by performing $L$ Fast Fourier Transformations with $\mathcal{O}(L^2 \ln L)$.

Figure: Husimi Functions of the coherent state $|0,0\rangle$ in phase space for different system sizes $L$ and unsharpness ratio $\sigma$. $Q$ is zero in the dark blue area and maximal in the red area. In the left picture $\sigma$ is nonsymmetric while it is symmetric in the other two.
Visualizing the metal-insulator-transition in phase space:

- $W = \lambda = 0$: electron describes a free wave
  $\implies$ momentum fully determined, but position arbitrary

- $W, \lambda$ very large: electron is localized at one lattice site
  $\implies$ momentum arbitrary, but position fully determined

- intermediate regime; $W, \lambda \approx O(1)$: versatile behaviour
  $\implies$ specific distribution patterns in phase space

- Anderson-Model: avoided crossings in energy spectrum $\Rightarrow$
  “jumping” between different eigenstates at intermediate $W$

- Aubry-André-Model: no avoided crossings $\Rightarrow$ always the same
  eigenstate

(next figure: Husimi Function of the Anderson-Model (top) and
Aubry-André-Model (below) at different disorder strengths)
Metal-Insulator Transition
Husimi Function
Monge Distance
Dynamics of the Zeros

Phase Space in Quantum Mechanics
Husimi Function
Zeros of the Husimi Function
Obtaining the Zeros Numerically

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The Husimi Function has been defined as

\[ Q(x, k) = |\langle x, k | \psi \rangle|^2 \]

where \( \langle x, k | \psi \rangle \) is the projection of \( |\psi\rangle \) onto a coherent state.

**Definition of the Bargmann Function:**

\[ B(x, k) = \langle x, k | \psi \rangle \]

- \( Q(x, k) = |B(x, k)|^2 \)
- \( Q \) is a real, positive-valued function while \( B \) is complex-valued
- correspondences:
  - \( B \cong \psi(x) \) (“wave function” in phase space)
  - \( Q \cong |\psi(x)|^2 \) (“probability” in phase space)
Properties of the Bargmann Function:

- $B(z)$ with $z = x + ik$ is periodic in phase space, but not analytic (i.e. complex differentiable)
- however, one can define $\tilde{B}(z) = B(z) \exp\left\{\pi L \left(\frac{|z|^2}{2} + ik\right)\right\}$
- $\tilde{B}$ is an analytic, but not periodic function
- results about $\tilde{B}$ can be obtained with complex analysis
- analogous definition of Husimi Function: $\tilde{Q} := |\tilde{B}|^2$
- Lebœuf and Voros found that $\tilde{B}$ has $L$ zeros and can be entirely constructed from its zeros by means of the Weierstrass-Hadamard Factorization
Factorization of the Bargmann Function:

\[ \tilde{B}(z) = Z \exp \left\{ \left( \pi \sum_{j=1}^{L} (\tilde{z}_j - \tilde{z}_0) \right) z \right\} \prod_{j=1}^{L} \tilde{B}_1(z + z_0 - z_j) \]

with the normalization factor \( Z \), the zeros \( z_1, z_2, \ldots, z_L \), and the middle point in phase space \( z_0 \).

- \( \tilde{B}_1(z) \), the “factor function”, is related to a Jacobian Theta Function and has its only zero at \( z_0 \)
- \( \tilde{B}_1(z) \) nearly radially symmetric \( \Rightarrow \) “generalization” of \((z - z_0)\)
- by definition, \( B, \tilde{B}, Q \) and \( \tilde{Q} \) have the same zeros

\[ \Rightarrow \text{The Bargmann Function and equivalently the Husimi Function are completely determined by their zeros!} \]
How can the positions of the zeros be obtained in practice?

- analytical calculation of Husimi Function is too complex
- $\Rightarrow$ zeros have to be obtained from numerical results
- we know $L \times L$ values of $B$ (and thus of $Q$)

Two possible ways to extract the zeros:

1. Find the **minima** of the **Husimi Function**
2. Find the **complex angle curls** of the **Bargmann Function**
Minima of the Husimi Function:

- \( Q(z) \geq 0 \) for all \( z \in \mathbb{C} \)
- \( Q(z_i) = 0 \) for all zeros \( z_i \)

\[ \Rightarrow \text{all zeros are minima} \]

Are all minima zeros, too?

No proof for this, but all results indicate: “Yes”

- Composition of \( Q \) from elementary “radial” functions \( \widetilde{B}_1(z) \) makes additional minima seem rather unlikely
- For a vast number of numerically examined Husimi Functions all minima have been verified as zeros (with the second method)
- Visualization of the Husimi Function on a logarithmic scale reveals a very “good-natured” and smooth behaviour
Figure: Left: Husimi Function on a linear scale. The positions of the zeros are indicated by crosses. Right: The same Husimi Function on a logarithmic scale where white points indicate the zeros. Note the smoothness and the fact, that there are no bright spots in the right picture that aren’t marked as zeros in the left picture.
Figure: Zeros that are close to each other may not be detected separately, if the resolution of the numerical data is too low.
Curls in the complex phase of the Bargmann Function:

- $B(z)$ is complex $\Rightarrow B(z) = R(z) e^{i\varphi(z)}$
- consider only the complex phase $\varphi(z) \in [0, 2\pi)$

Weierstrass-Hadamard Factorization $\Rightarrow \varphi(z)$ covers the whole codomain near every zero

$\Rightarrow$ zeros can be obtained reliably by finding the curls of $\varphi(z)$

(next figure: complex phase $\varphi(z)$ of a Bargmann Function, drawn with a cyclic color palette)
numerical detection of curls:
check the monotonicity of 4 adjacent sample points
- all zeros are detected (at least usually)
- many false positive results
⇒ tighten the detection condition by requesting an additional "smoothness condition" for the curl
⇒ together, these methods allow for a reasonably good detection of all $L$ zeros

(next figure: Left picture shows complex phase $\varphi(z)$, upper right shows many false positive detection results, lower right shows too strict "smoothness conditions". In all pictures, the zeros are marked with circles.)
Metal-Insulator Transition
Husimi Function
Monge Distance
Dynamics of the Zeros

Phase Space in Quantum Mechanics
Husimi Function
Zeros of the Husimi Function
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\[ \pi \]
\[ k \]
\[ 0 \]
\[ 0 \]
\[ L \]
\[ x \]

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How to quantify the dynamical changes of the Husimi Function?

**Idea:** Define a measure of distance between two Husimi Functions!

1:1 correspondence between $|\psi\rangle$ and $Q$ enables us to employ well known Density Operator Measures for this, e.g.

- **Trace Distance:**
  
  $$D_{tr}(\rho_1, \rho_2) = \text{tr}\sqrt{(\rho_1 - \rho_2)^2}$$

- **Hilbert-Schmidt Distance:**
  
  $$D_{HS}(\rho_1, \rho_2) = \sqrt{\text{tr}\left[(\rho_1 - \rho_2)^2\right]}$$

**Problem:** They don’t account for the shape of Husimi Functions.

**Example:** “semiclassical property” for coherent states not fulfilled:

$$D(|\alpha_1\rangle, |\alpha_2\rangle) \neq |\alpha_1 - \alpha_2|$$
Monge-Problem (1781): How to move a pile of sand from one location to another with the smallest possible effort?

Mathematically: Find a map $T : Q_1 \rightarrow Q_2$ between the grains of sand of the two piles so that the transportation effort is minimized!
Definition of the Monge Distance:

\[ D_M(Q_1, Q_2) = \inf \int_{\mathbb{R}^d} |x - T(x)| Q_1(x) \, d^n x \]

- the map \( T \) “distorts” the plane so that \( Q_1 \) is mapped to \( Q_2 \)
- \( |x - T(x)| \) denotes the transportation distance
- infimum is taken over all the \( T \) that map \( Q_1 \) to \( Q_2 \)
How to evaluate this formula for two given Husimi Functions?

- evaluation of integral is too complex!
- simple-form analytical solutions exist only for 1D systems
How to evaluate this formula for two given Husimi Functions?

- evaluation of integral is too complex!
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⇒ make a simplification:

replace the continuous $Q_i$ with a discrete approximation:

$$Q_i \longrightarrow \sum_{j=1}^{N} Q_i(x_j) \delta(x - x_j)$$

- the sampling points $\{x_j\}$ are chosen to reflect the shape of $Q_i$
- **but**: many sampling points needed for precise modeling of $Q_i$
⇒ make an even further simplification:

Życzkowski et al.: for pure states the Husimi Function can be associated with a discrete distribution consisting of the Husimi Zeros:

\[ |\psi\rangle \rightarrow f_\psi(x) := \frac{1}{N} \sum_{i=1}^{N} \delta(x - x_i) \]

This yields the simplified Monge Distance:

\[ D_{sM}(|\psi\rangle, |\Phi\rangle) := D_M(f_\psi, f_\Phi) \]

The Monge Problem has now been reduced to finding the “shortest way”-map between the zeros of two Husimi Functions.
two zero distributions with $L$ zeros each $\Rightarrow L!$ possible mappings

- simply trying out all possibilities requires exponential time
- efficient algorithms for finding the optimal mapping do exist!
two zero distributions with $L$ zeros each $\Rightarrow L!$ possible mappings

- simply trying out all possibilities requires exponential time
- efficient algorithms for finding the optimal mapping do exist!

The theory of **Linear Programming** provides efficient algorithms for many classes of problems. Two important classes are:

- **Assignment Problems:**
  $N$ items have to be transported from initial locations to final locations – how to transport them most efficiently?

- **Transportation Problems:**
  Each one of $A$ suppliers possesses $a_i$ items and each one of $B$ destinations requires $b_i$ of the items.

**Monge problem $\in$ Assignment Problems $\subset$ Transportation Problems**
Two algorithms are suitable for the Monge Problem:

- **Simplex Algorithm**

- **Hungarian Method**
Two algorithms are suitable for the Monge Problem:

- **Simplex Algorithm**
  - well known and well documented
  - for *Transportation Problems* ⇒ very general algorithm
  - usually fast, but exponential in the worst case

- **Hungarian Method**
  - not well known and scarcely documented
  - for *Assignment Problems* ⇒ specialised algorithm
  - very fast, run time never exceeds $O(L^3)$

⇒ for speed and reliability, the **Hungarian Method** was chosen
from the problem to the algorithm:

Example:

- two Husimi Functions with 3 zeros each
- left figure: shortest path from zero $i$ of first distribution to zero $j$ of second distribution is denoted by $a_{ij}$
- right figure: optimal map (the “Monge Plan”) is shown
**Algorithmic approach:**

- determine the matrix of the distances \( \{a_{ij}\} \) with \( a_{ij} \geq 0 \)

**Observations:**

- in every row and column, there is *one* entry that belongs to the Monge Plan
- changing the values of a row or column by a constant doesn’t change the Monge Plan
Algorithmic approach:

- determine the matrix of the distances \( \{a_{ij}\} \) with \( a_{ij} \geq 0 \)

Observations:

- in every row and column, there is one entry that belongs to the Monge Plan
- changing the values of a row or column by a constant doesn’t change the Monge Plan

Basic idea: find the Monge Plan by appropriately subtracting constants from rows and columns such that

- as many matrix entries as possible become 0
- no matrix entry becomes negative

If one 0 can be chosen from every row and every column, then these 0’s denote the Monge Plan!
The Hungarian Method is basically a prescription telling us which values to subtract from which row/column, in order to find the desired formation of 0’s within $\mathcal{O}(L^3)$ steps.

There are two common versions of the Hungarian Method in the literature. One of the two is often stucked in an infinite loop when applied to large matrices, thereby never terminating.

Gladly, the other version is sane and always terminates in polynomial time.
Dynamics of the Zeros

Until now:

- physical system of interest and its models were presented
- theory of Husimi Function and its zeros has been covered
- numerical extraction of the Husimi Zeros has been discussed
- a useful quantitative tool, the Monge Distance, was introduced
Dynamics of the Zeros

Until now:

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Now tackling:

Qualitative and quantitative analysis of the dynamics of the Husimi Zeros when varying the disorder potential.

- similarities and differences between Anderson-Model and Aubry-André-Model?
- how are the dynamics of the Husimi Function and of the Husimi Zeros related?
Analysis of the qualitative behaviour:

low disorder regime:

- in the beginning all zeros are aligned along two horizontal lines
- vertical movement of the zeros into phase space when increasing $\mathcal{W}$, $\lambda$
- at $\mathcal{W}$, $\lambda \approx 1$ nearly the whole phase space is covered

Aubry-André:

- several movement lines
- all zeros lie at one of the movement lines
- zeros of one line are equidistant

Anderson:

- only foremost movement lines
- zeros remaining behind the movement lines no longer move
top row: Aubry-André-Model

bottom row: Anderson-Model

a) $\lambda = 10^{-12}$

b) $\lambda = 10^{-10}$

c) $\lambda = 10^{-6}$

d) $\lambda = 10^{-2}$

e) $\lambda = 10^{0}$

f) $W = 10^{-12}$

g) $W = 10^{-10}$

h) $W = 10^{-6}$

i) $W = 10^{-2}$

j) $W = 10^{0}$

Metal-Insulator Transition
Husimi Function
Monge Distance
Dynamics of the Zeros

Nearest Neighbor Statistics
Monge Distance Statistics
Conclusion
transition regime:

- movement changes from vertical to horizontal
- at one point, the entire phase space is covered by zeros
- Aubry-André:
  - zeros possess a distinct ordering pattern
  - transition from momentum to position localization occurs fast
- Anderson:
  - no distinct ordering pattern recognizable
  - chaotic shuffling of the zeros due to avoided crossings
  - transition takes place over broader interval of disorder strength
top row: Aubry-André-Model

bottom row: Anderson-Model

\[\begin{array}{cccccc}
\text{a) } \lambda = 0, 1 & \text{b) } \lambda = 1 & \text{c) } \lambda = 2 & \text{d) } \lambda = 4 & \text{e) } \lambda = 10 \\
\text{f) } W = 0, 1 & \text{g) } W = 1 & \text{h) } W = 2 & \text{i) } W = 4 & \text{j) } W = 10 \\
\end{array}\]
high disorder regime:

- zeros form vertical lines in the high disorder limit
- Aubry-André:
  - position localization quickly finished
- Anderson:
  - position localization takes long time
  - not all zeros move to vertical lines; some remain scattered
  - scattering changes permanently and in a nonpredictable way
top row: Aubry-André-Model

bottom row: Anderson-Model

- **f)** $W = 2$
- **g)** $W = 10$
- **h)** $W = 20$
- **i)** $W = 100$
- **j)** $W = 1000$

- **a)** $\lambda = 2$
- **b)** $\lambda = 2.5$
- **c)** $\lambda = 3$
- **d)** $\lambda = 6$
- **e)** $\lambda = 10$
relationship between Husimi Function and Husimi Zeros:

- Zeros change on a logarithmic scale while $Q$ changes on a linear scale
- Similarly widespread zeros during the transition in both models, but very different shapes of Husimi Function
- Anderson: rapid scattering of zeros for big $W$ doesn’t affect shape of Husimi Function
Nearest Neighbor Statistics:

- nearest neighbors of all zeros can be quickly calculated: $O(L^2)$
- distribution $P(x)$ of nearest neighbor distances is obtained
- integrated distribution: $I(x) = \frac{1}{L} \int_{0}^{x} dx' P(x')$
- $I(x) \in [0, 1]$ can be used to visualize the dynamics of the nearest neighbor statistics

(next figure: $I(x)$ of a Husimi Function of the Anderson-Model and of the Aubry-André-Model. $I(x)$ is color-coded: $I(x) = 0$ for red and $I(x) = 1$ for blue.)
Anderson-Modell

Aubry-André-Modell

Potenzialstärke $W$

Potenzialstärke $\lambda$
Metal-Insulator Transition
Husimi Function
Monge Distance
Dynamics of the Zeros

Qualitative Behaviour
Nearest Neighbor Statistics
Monge Distance Statistics
Conclusion

\[ \lambda = 0,5 \]
\[ \lambda = 1,3 \]
\[ \lambda = 2 \]
\[ \lambda = 9 \]

[Graph showing data distribution]
Monge Distance Statistics:

- determine the Husimi Zeros for equidistant $\lambda$ on the logarithmic scale
- find the Monge Distance between all pairs of adjacent sample values of $\lambda$
- plotting the results, one can see how fast the Husimi Zeros change at different $\lambda$
Figure: Monge Distance plot of the Husimi Zeros of the Anderson-Model (left) and of the Aubry-André-Model (right). The large and rapidly changing values on the left are reminiscent of the avoided crossings. Also, the fuzzy curve for high $W$ is a result of the rapid scattering of some zeros in the Anderson-Model.
Figure: Transition area $\lambda \approx 2$ of the same Husimi Function of the Aubry-André-Model as in the last figure.
Conclusion

- close relationship between periodic $B$ and analytic $\tilde{B} \Rightarrow$
  complex analysis yields results about Bargmann Function
- $Q$ is completely determined by its zeros $\Rightarrow$
  “the zeros of $Q$ contain the physics of $Q$ itself”
- numerically obtained minima always verified as zeros
  $\Rightarrow$ Are all minima of $Q$ zeros? How to proof this?
- nearest-neighbor-distribution elucidates the phase transition
- Monge Distance is an excellent tool for detecting the phase transition of the Aubry-André-Model