

Quantum Mechanics in Discrete Phase-Space

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Caos y Complejidad

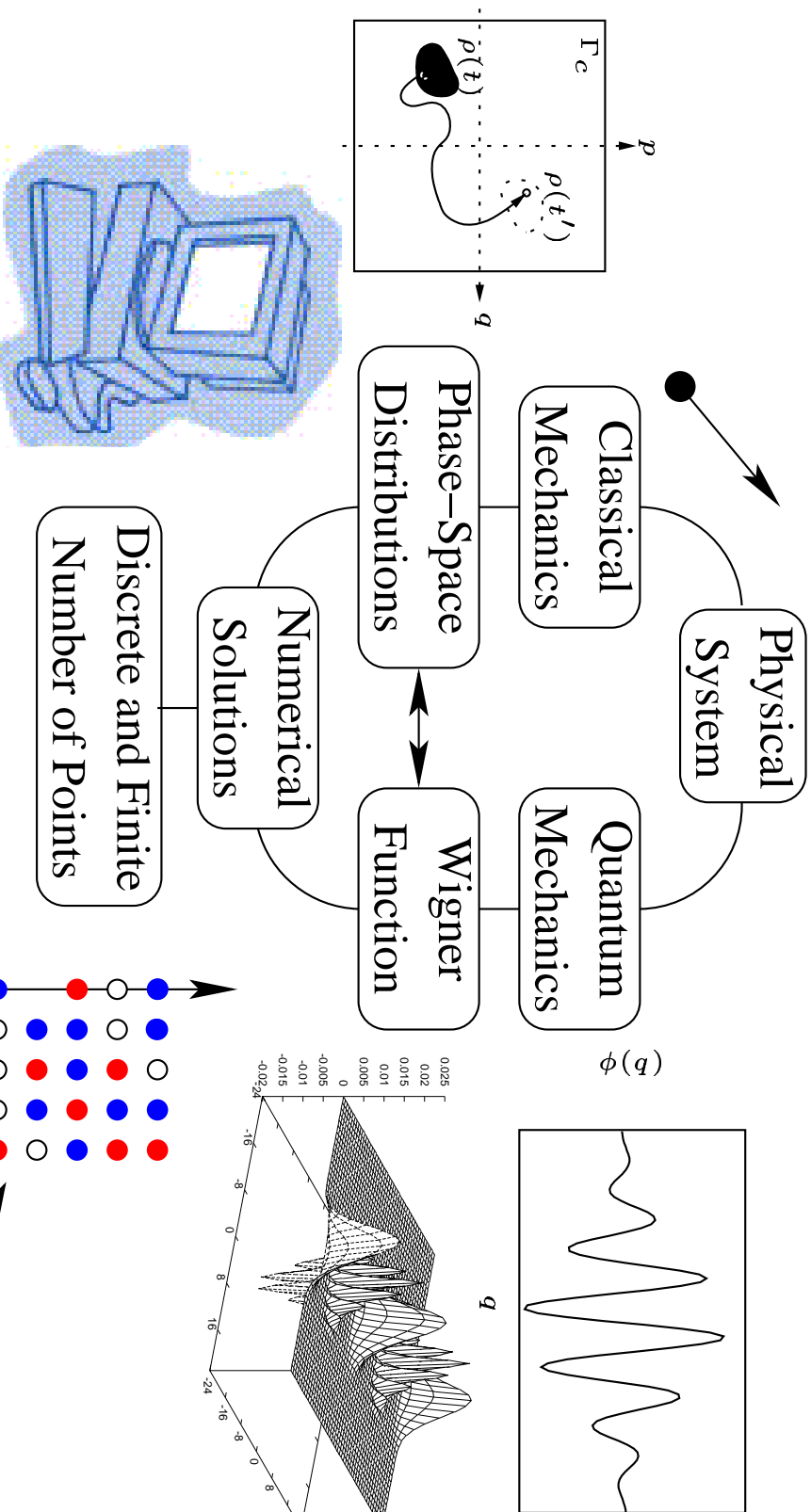
Departamento de Física

Facultad de Ciencias



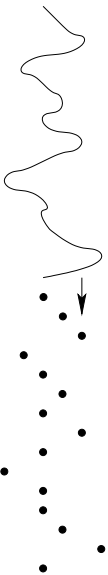
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Motivation

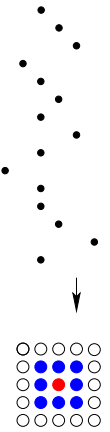


1. Objectives

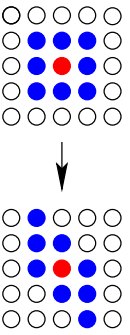
1. Analyze consequences of discretization.



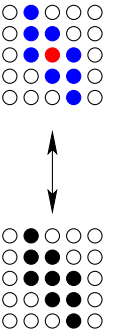
2. Construct a well-defined discrete Wigner function.



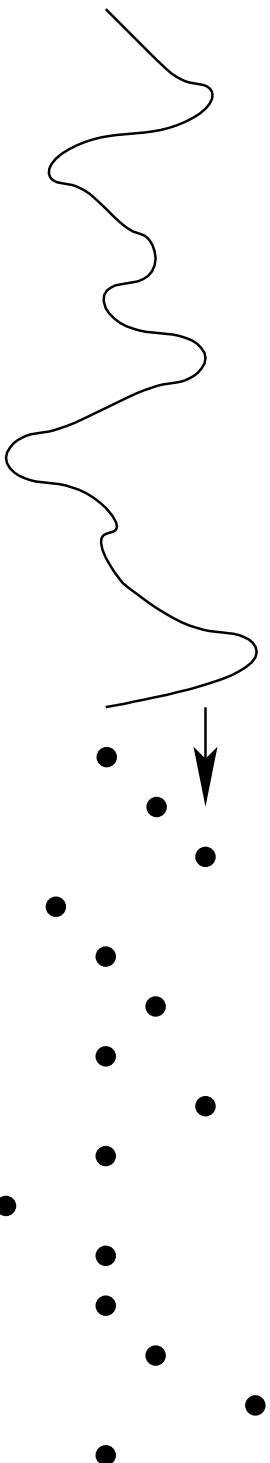
3. Use this formulation to calculate the quantum time evolution.



4. Compare classical and quantum results for several examples.



2. Periodic & Discrete



2. Periodic & Discrete

In quantum mechanics the position and momentum matrix elements transformation are given by

$$\langle p|q\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipq/\hbar}.$$

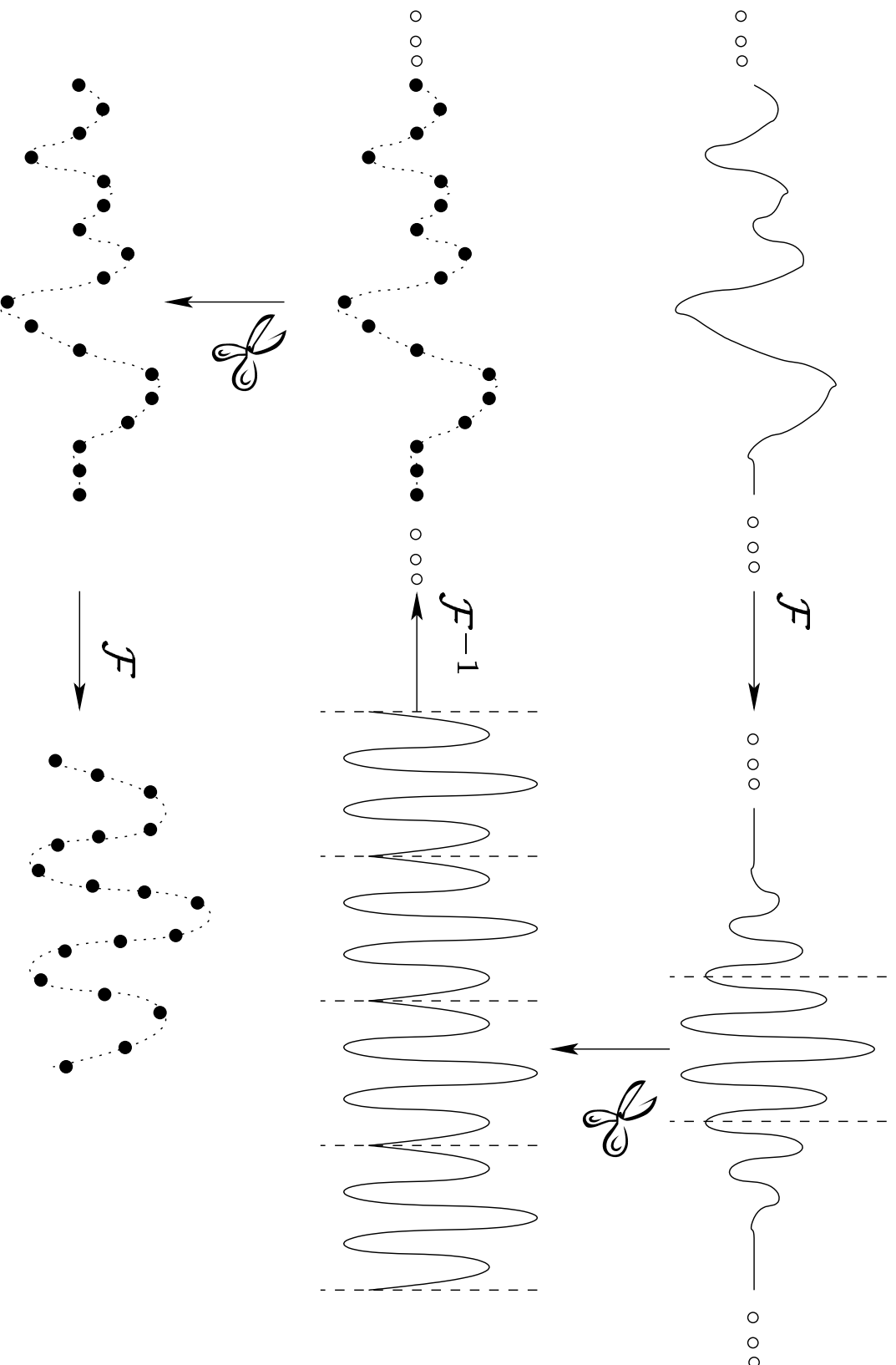
Therefore, the relation is a Fourier transformation.

The Wigner function is defined as

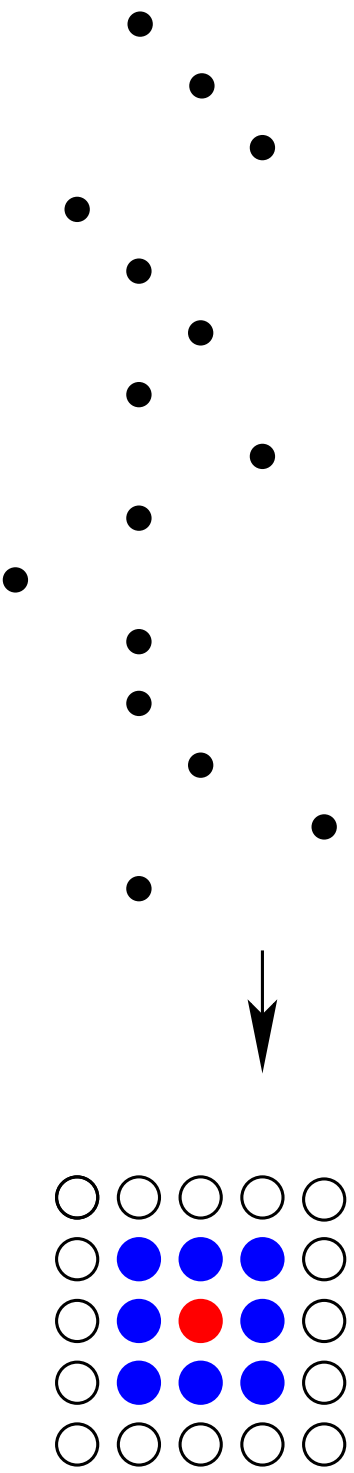
$$\rho_w(p, q) = \frac{1}{2\pi\hbar} \int dq' \langle q + q'/2 | \hat{\rho} | q - q'/2 \rangle \exp(-ipq'/\hbar),$$

where there appears a Fourier transformation as well.

2. Periodic & Discrete



3. The Discrete Wigner Function



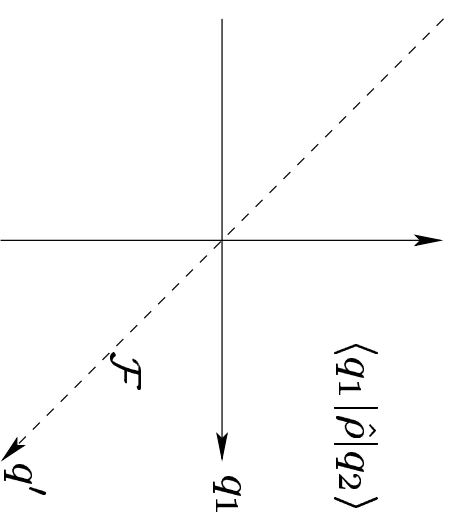
3. The Discrete Wigner Function

From the definition $\rho_w(p, q) = \frac{1}{2\pi\hbar} \int dq' \langle q + q'/2 | \hat{\rho} | q - q'/2 \rangle \exp(-ipq'/\hbar)$, we can see that the Wigner function is a Fourier transformation of the density operator along an inclined axe. Defining

$$q_1 = q + q'/2, \quad q = (q_1 + q_2)/2,$$

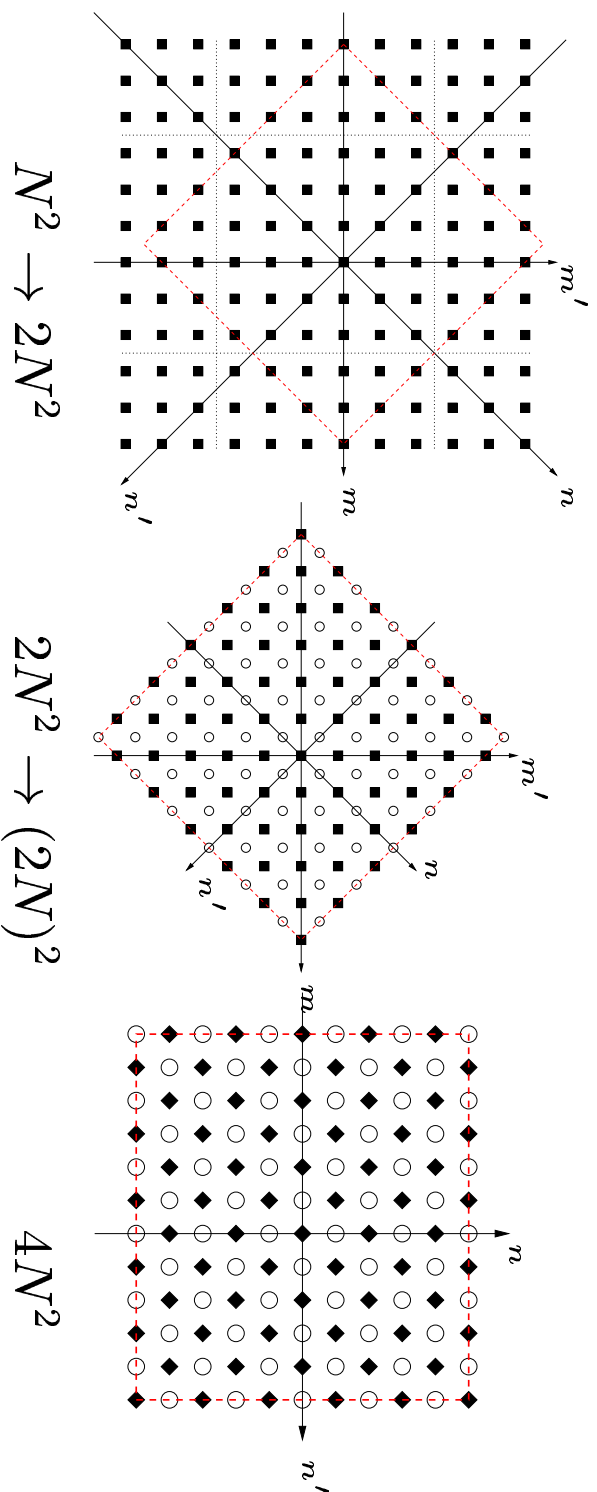
$$q_2 = q - q'/2, \quad q' = q_1 - q_2;$$

we have

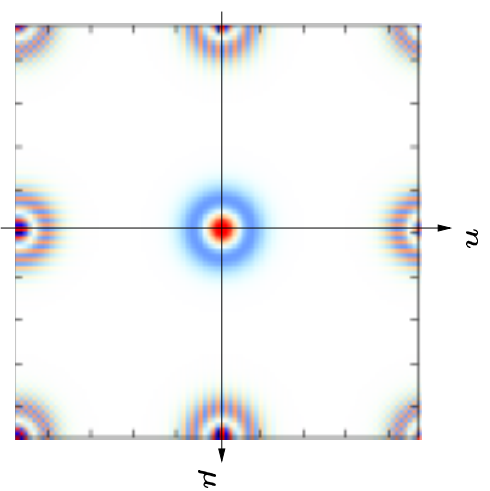
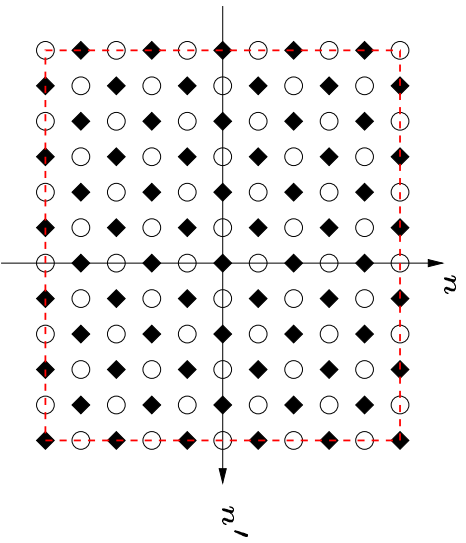
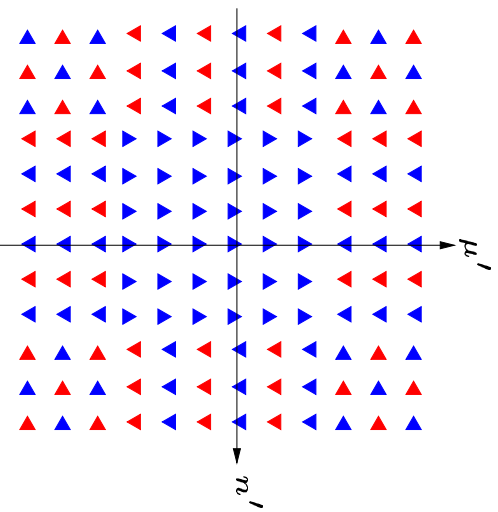


In the case of a discrete space, we have $q_m = mQ/N$, $p_\mu = \mu P/N$ and $N = QP/2\pi\hbar$, where Q and P are the period in space and momentum respectively.

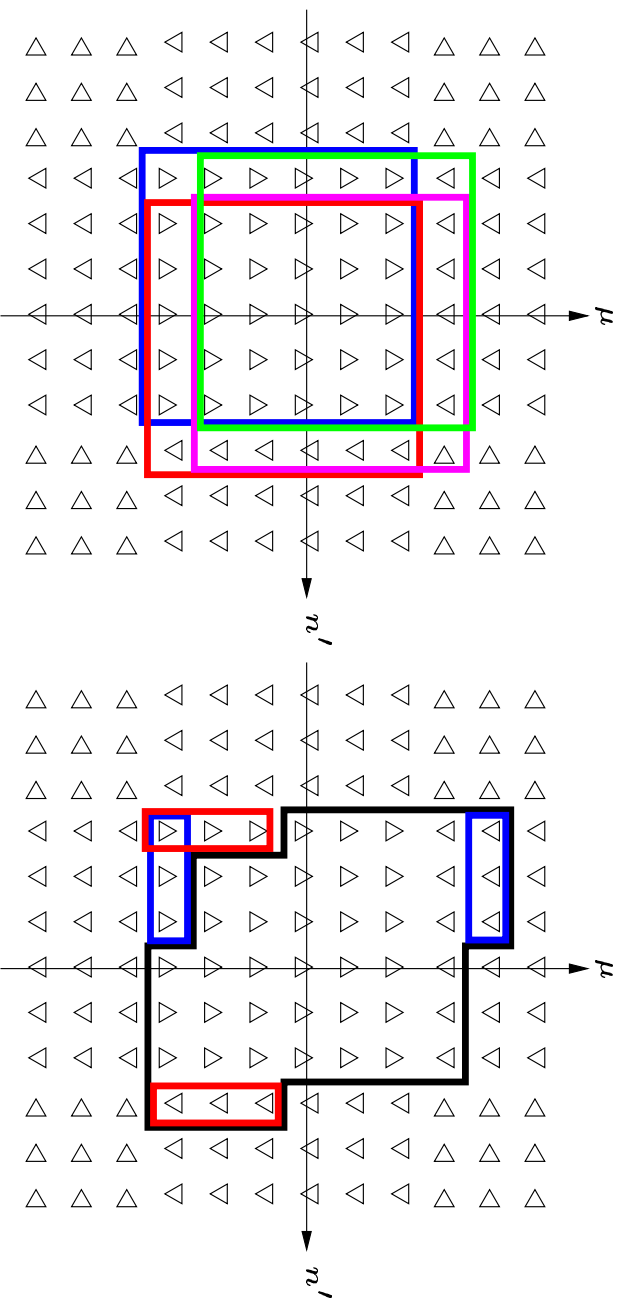
3. The Discrete Wigner Function



3. The Discrete Wigner Function



3. The Discrete Wigner Function



3. The Discrete Wigner Function

Finally, the discrete Wigner function is given by the expression

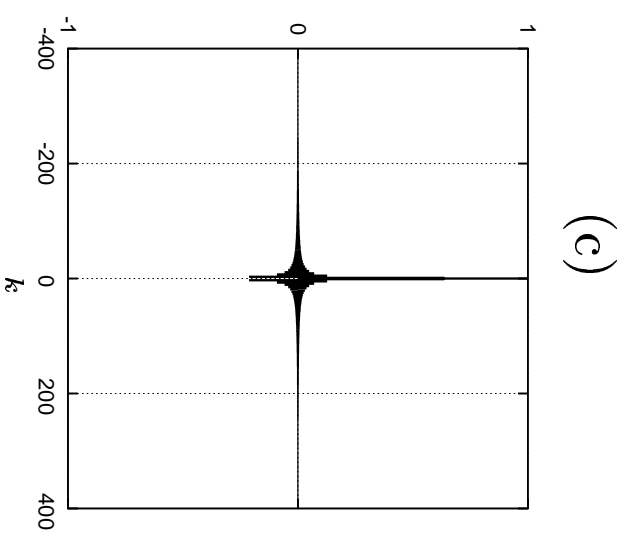
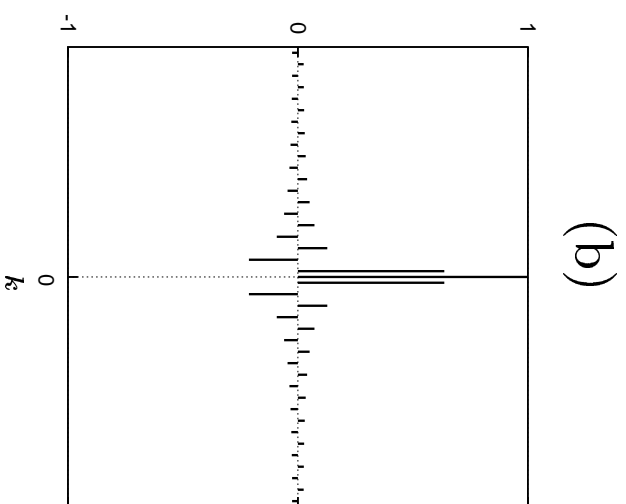
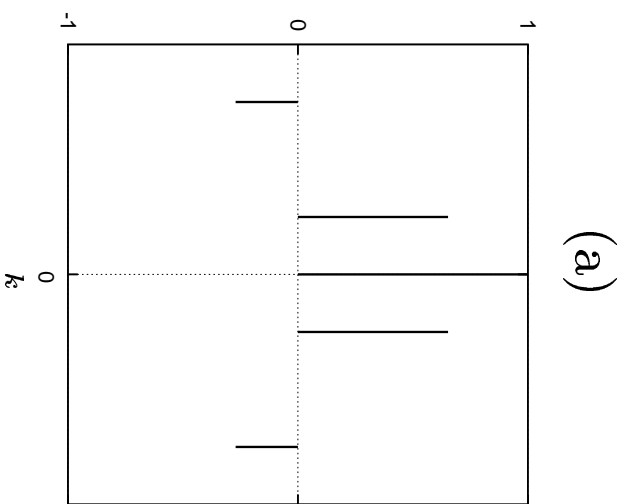
$$\rho_w(p_\mu, q_n, t) = \frac{1}{N} \sum_{n'} \sum_n^{2N} \delta_n^{n'} \left\langle \frac{n+n'}{2} \left| \hat{\rho}(t) \right| \frac{n-n'}{2} \right\rangle \tilde{\delta}(2m-n) e^{-2i\pi \frac{n'\mu}{N}},$$

where

$$\delta_n^{n'} = \frac{1 + (-1)^{n+n'}}{2}, \quad \tilde{\delta}(k) = \frac{1}{N} \frac{\sin(\pi k/2)}{\sin(\pi k/2N)};$$

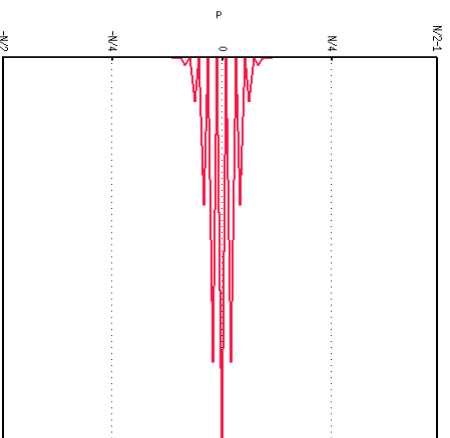
with the property $\tilde{\delta}(2k) = \delta(k)$. One can prove that

- ρ_w is real.
- $\sum_m \rho_w(\mu, m) = \langle \mu | \hat{\rho} | \mu \rangle$, $\sum_\mu \rho_w(\mu, m) = \langle m | \hat{\rho} | m \rangle$.
- $\sum_{\mu m} \rho_w(\mu, m) A_w(\mu, m) = \text{Tr}[\hat{\rho} \hat{A}]$

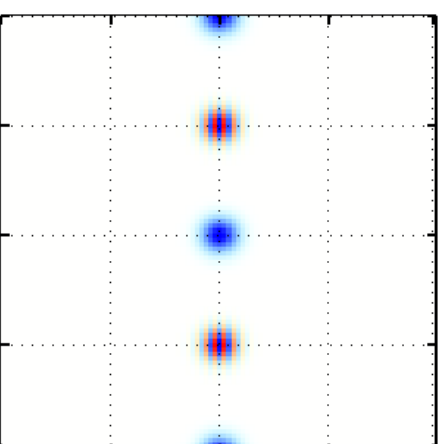


$\tilde{\delta}(k)$ plots for (a) $N = 4$, (b) $N = 40$ and (c) $N = 400$.

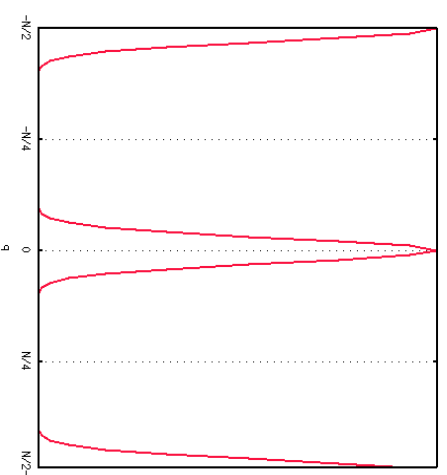
3. The Discrete Wigner Function



$$\sum_q \rho_w(p_\mu, q_m)$$

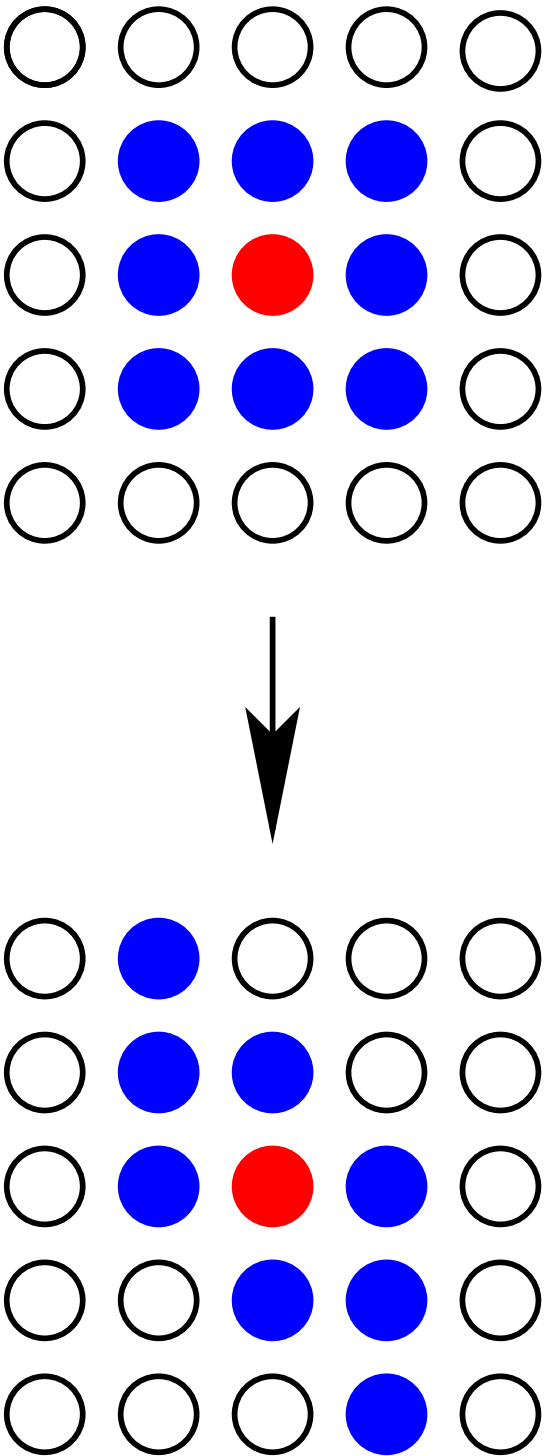


$$\rho_w = \mathcal{T}[\hat{\rho}]$$

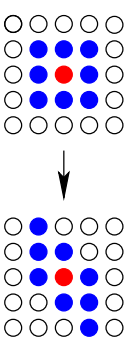


$$\sum_p \rho_w(p_\mu, q_m)$$

4. Time Evolution



4. Time Evolution



In order to perform the quantum time evolution:

- Take a basis on the quantum Hilbert space.
- Rewrite the Weyl transformation of the density matrix using the choosed basis.
- Use the quantum time evolution operator to calculate the density matrix at time t' from t .

4. Time Evolution

We can use the set of eigenvalues of an operator as a basis for the Hilbert space and for the space of linear operators on this Hilbert space, for example choosing the energy eigenstates $\hat{H}|\phi_a\rangle = E_a|\phi_a\rangle$; therefore we have

$$|\psi\rangle = \sum_a \psi_a |\phi_a\rangle, \hat{A} = \sum_{ab} A_{ab} |\phi_a\rangle\langle\phi_b|;$$

where $\psi_a = \langle\psi|\phi_a\rangle$ and $A_{ab} = \langle\phi_a|\hat{A}|\phi_b\rangle$.

The $\{|\phi_a\rangle\}$ form a complete and orthonormal basis,

$$\hat{I} = \sum_a |\phi_a\rangle\langle\phi_a|, \langle\phi_a|\phi_b\rangle = \delta(a-b).$$

4. Time Evolution

In the case of the quantum phase-space, one can choose the Weyl transform of the operator basis $\mathcal{T}[|\phi_a\rangle\langle\phi_b|] = \Phi_{ab}(p_\mu, q_m)$, and we have

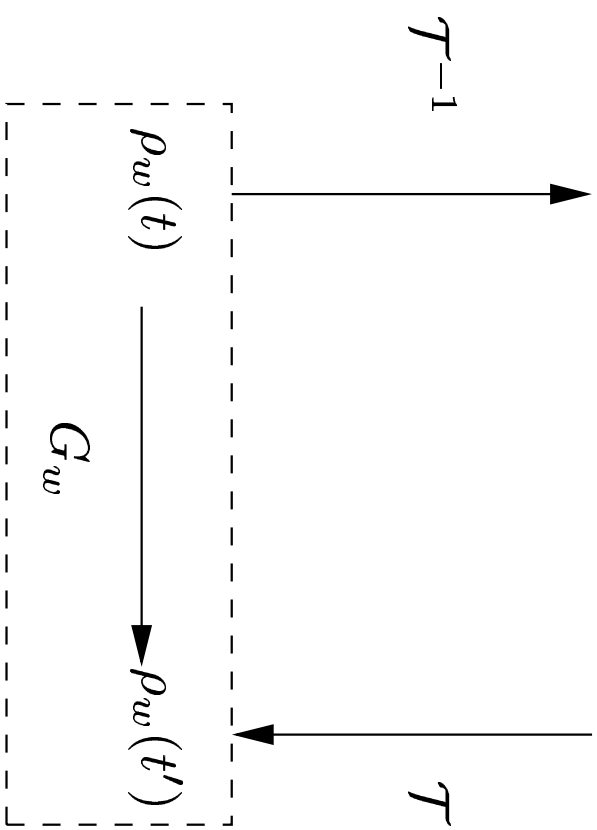
$$\sum_a \Phi_{aa}(p_\mu, q_m) = 1,$$

$$\frac{1}{N} \sum_{\mu m} \Phi_{ab}(p_\mu, q_m) \Phi_{cd}^*(p_\mu, q_m) = \delta(a - c) \delta(b - d);$$

These are the completeness and orthogonality relations in phase-space.

From the phase-space basis and

$$\hat{\rho}(t) \xrightarrow{\hat{U}(t', t)} \hat{\rho}(t')$$



we can rewrite the Wigner function at t' using the Wigner function at another time t as

$$\rho_w(t') = \mathcal{T}[U(t', t)\mathcal{T}^{-1}[\rho_w(t)]U^\dagger(t', t)]; \quad t, t' \in \mathcal{R}$$

4. Time Evolution

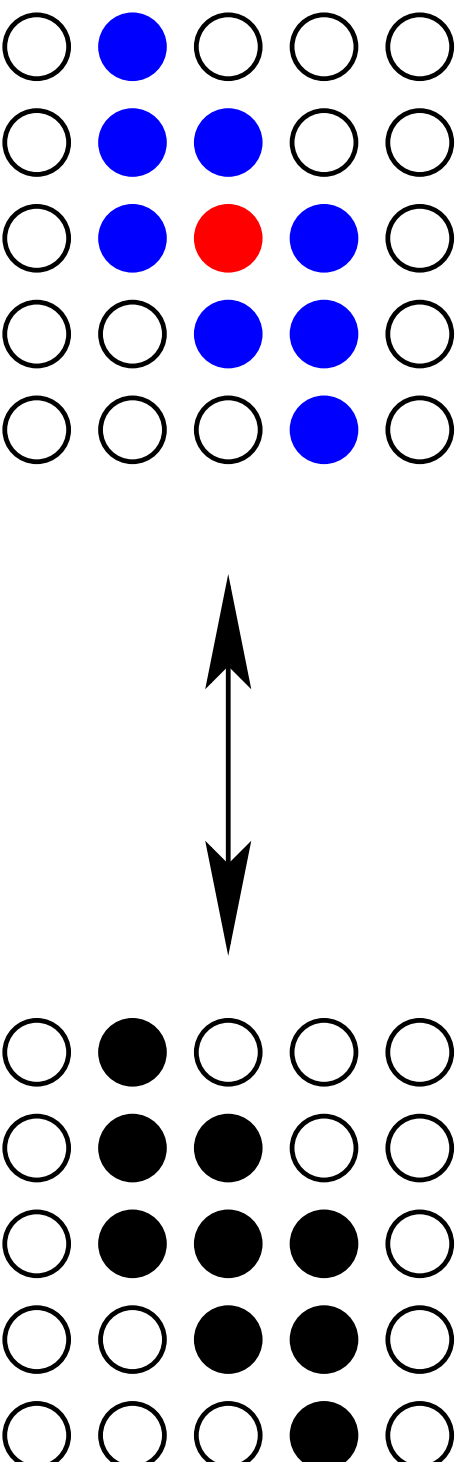
Therefore, the Wigner function propagator is given by

$$G_w(\mathbf{r}', t'; \mathbf{r}, t) = \frac{1}{N} \sum_{ab} e^{-\frac{i}{\hbar}(E_a - E_b)(t' - t)} \Phi_{ab}^*(\mathbf{r}) \Phi_{ab}(\mathbf{r}'),$$

where $\mathbf{r} = (p_\mu, q_m)$. The properties of the propagator are

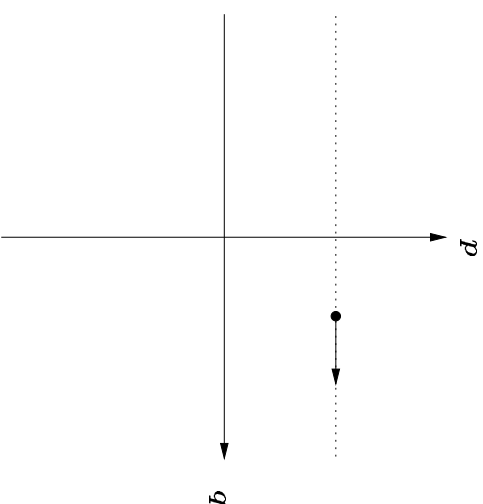
- It is real.
- $G_w(\mathbf{r}', t'; \mathbf{r}, t) = \delta(\mu' - \mu) \delta(m' - m)$.
- $G_w(t'', t) = G_w(t'', t') \circ G_w(t', t)$.
- $G_w^{-1}(t', t) = G_w(t, t')$.

5. Classical and quantum comparisons



5. Classical and quantum comparisons

Free Particle



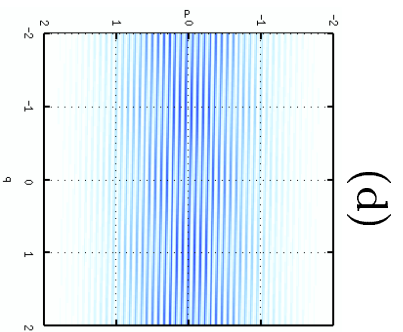
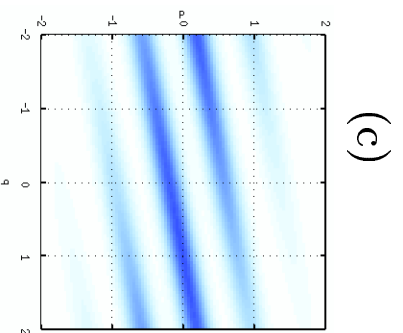
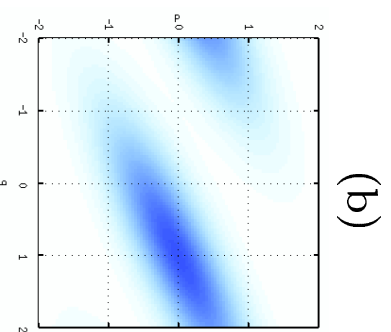
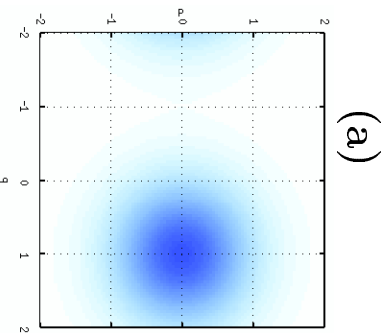
The classical propagator of a free particle is given by

$$G_c(p', q', t'; p, q, t) = \delta(p' - p) \delta(q' - q + p(t' - t)/m).$$

Thus, for a periodic system the distribution in t' is

$$\rho_c(p, q, t') = \rho_c(p \bmod P, (q - pt'/m) \bmod Q, 0).$$

Classical Free Particle



(a) $t = 0$ (b) $t = 1$, (c) $t = 5$ (d) $t = 50$. $m = 1$.

Quantum Free Particle

In the case of quantum mechanics, the eigenstates in coordinate representation are

$$\phi_p(q) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipq/\hbar}.$$

Imposing the periodicity with periods $P = Q = 1$, we have

$$\phi_\nu(m) = \frac{1}{\sqrt{N}} e^{2i\pi\nu m/N}.$$

These eigenstates allow us to calculate the Weyl basis functions

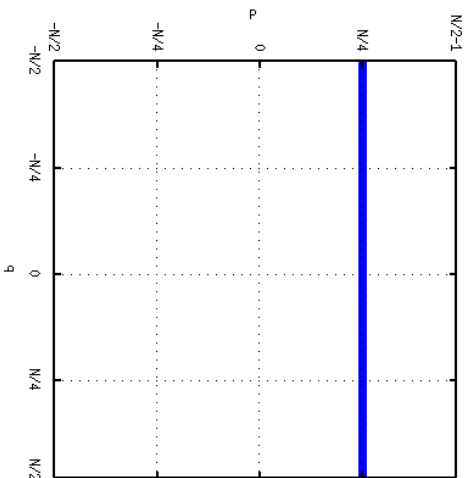
$$\Phi_{\nu\nu'}(\mu, m) = \frac{1}{N} e^{2i\pi m(\nu-\nu')/N} \tilde{\delta}(\nu + \nu' - 2\mu),$$

for $\text{par}(\nu) = \text{par}(\nu')$, $\bar{\nu} = (\nu + \nu')/2$ and $\Delta\nu = \nu - \nu'$ it is

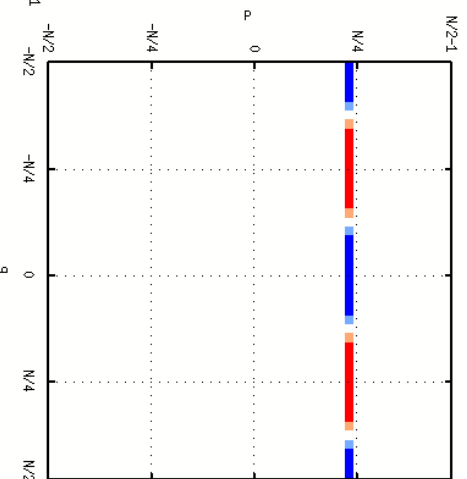
$$\Phi_{\nu\nu'}(\mu, m) = \frac{1}{N} e^{2i\pi m\Delta\nu/N} \delta(\bar{\nu} - \mu),$$

Quantum Free Particle- $\Phi_{\nu\nu'}(\mu, m)$

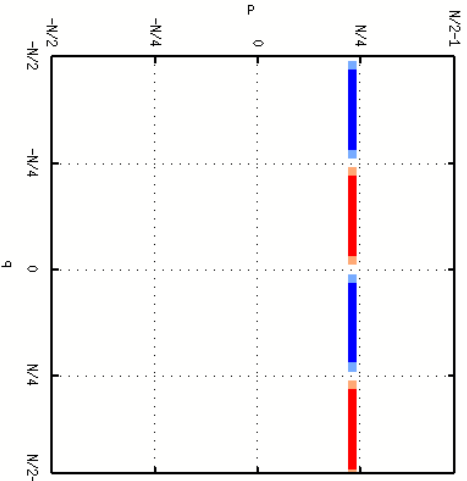
(a)



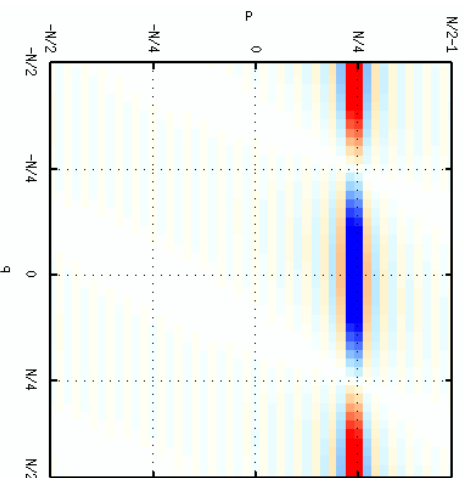
(b1)



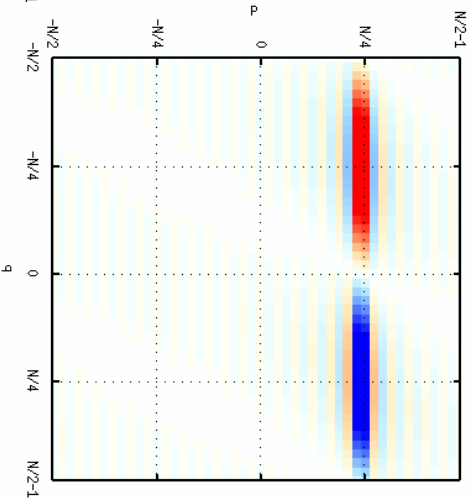
(b2)



(c1)

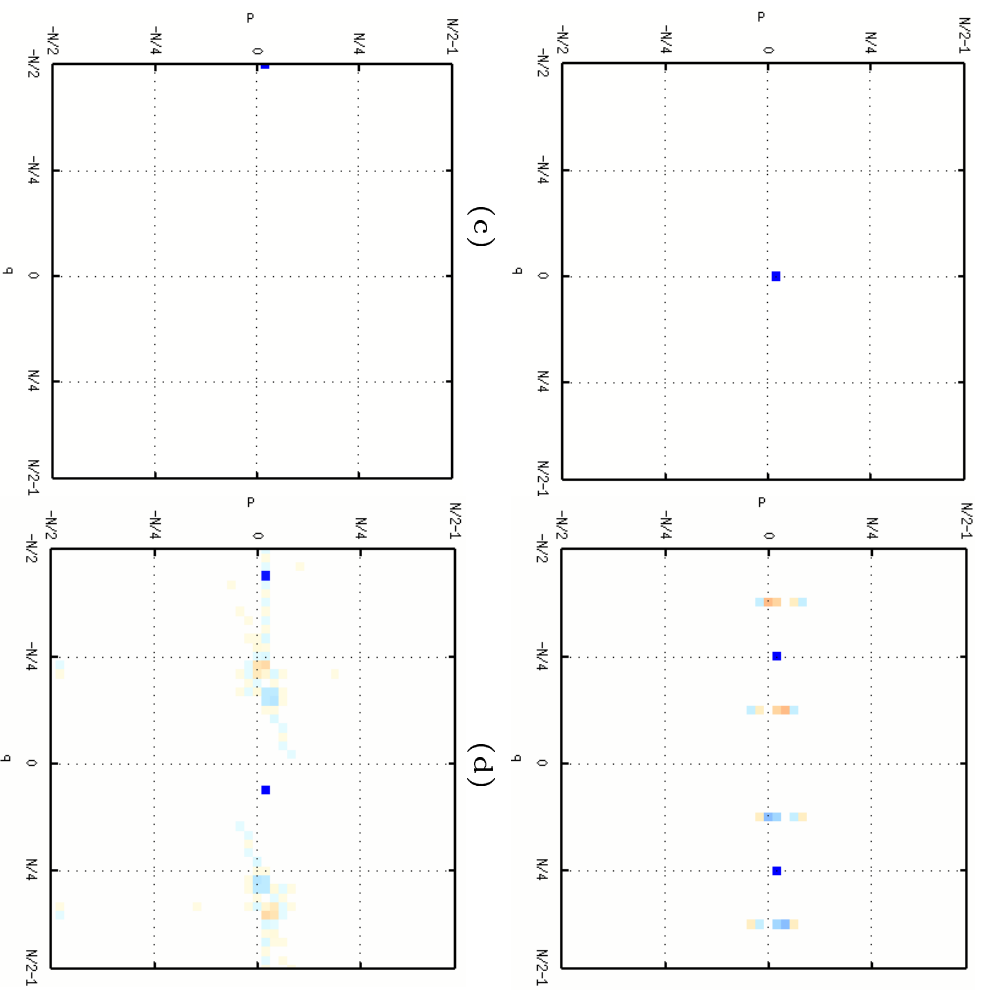


(c2)



(a) $\nu = \nu' = N/4$ (b) $\Phi_{12,10}$ (c) $\Phi_{12,11}$ (1) real part (2) imaginary part. $N=48$

Quantum Free Particle-Propagator



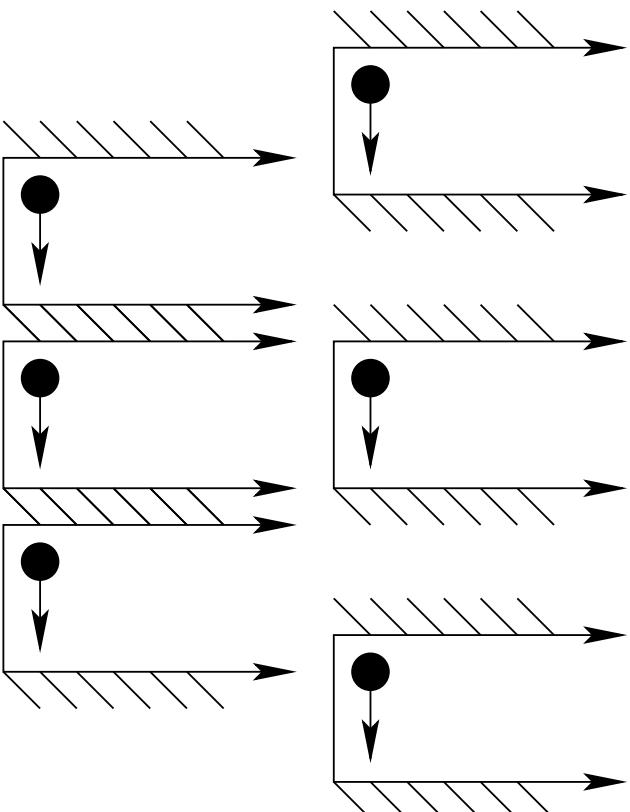
Wigner Function Propagator for $\mu = 1$, $m = 0$, $t = 0$, $N = 48$ and (a) $t' = 0$, (b) $t' = N/4$, (c)

$$t' = N/2 \text{ y (d) } t' = 52.$$

5. Classical and quantum comparisons

Delta spike model

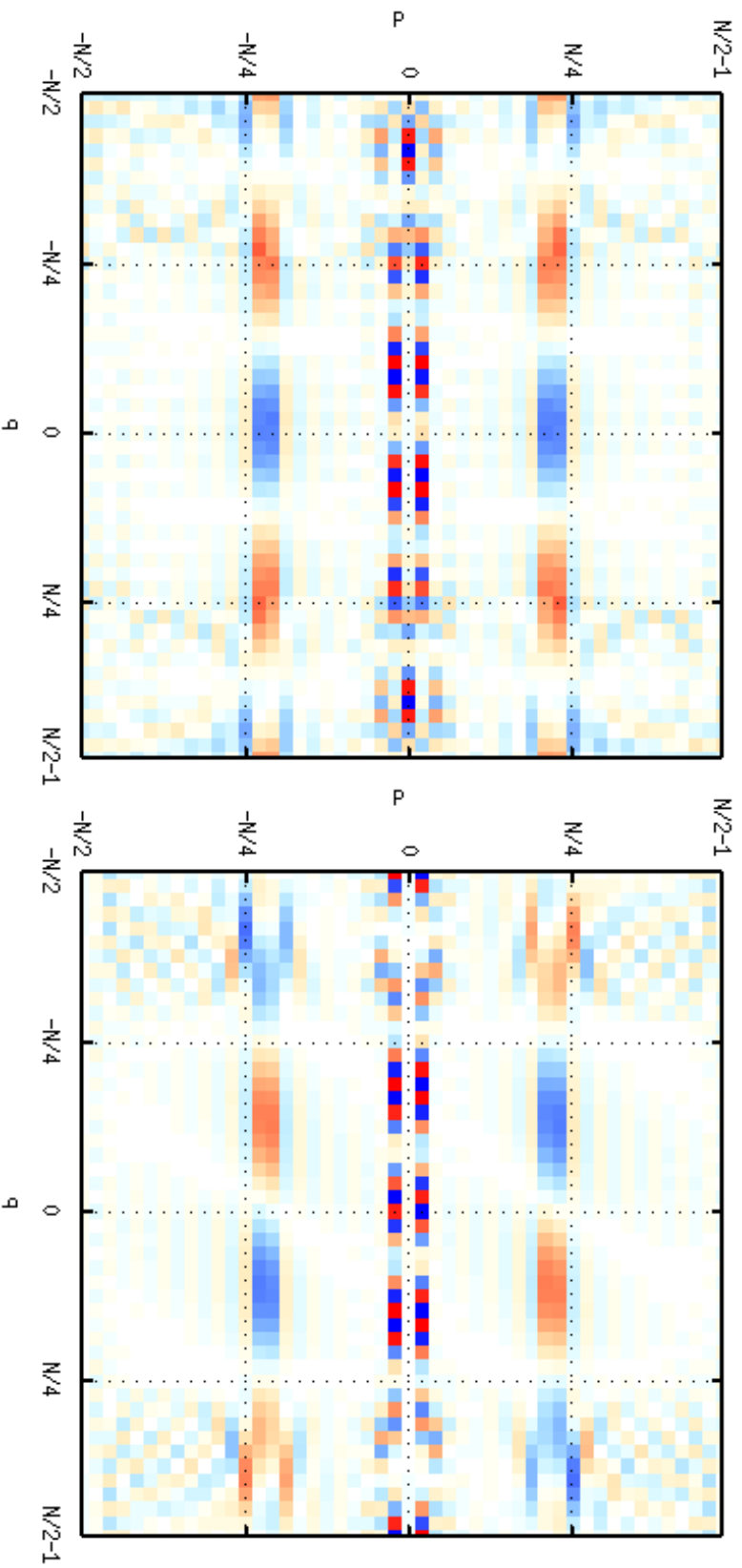
The scheme of the system is



Taking the discretization into account, the eigenfunctions are

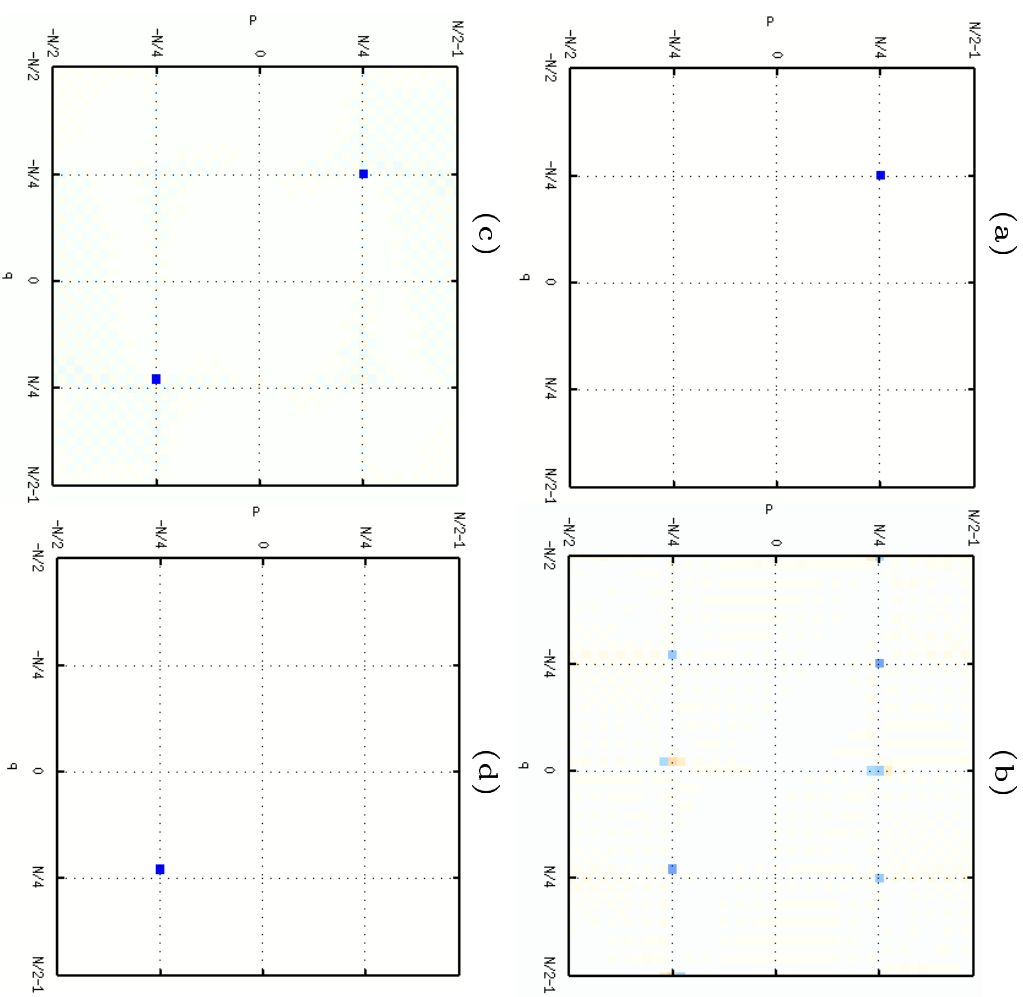
$$\Phi_\nu(n) = \begin{cases} \sqrt{\frac{2}{N}} \sin(\pi\nu(n - 1/2)/N) & \text{for } \nu = 1, \dots, N - 1, \\ \sqrt{\frac{1}{N}} \sin(\pi(n - 1/2)) & \text{for } \nu = N. \end{cases}$$

The analytical calculation of phase-space basis is more complex than the previous case. Then we use the numerical tool in order to calculate the propagator.



$$\Phi_{29-25}(\mu, m)$$

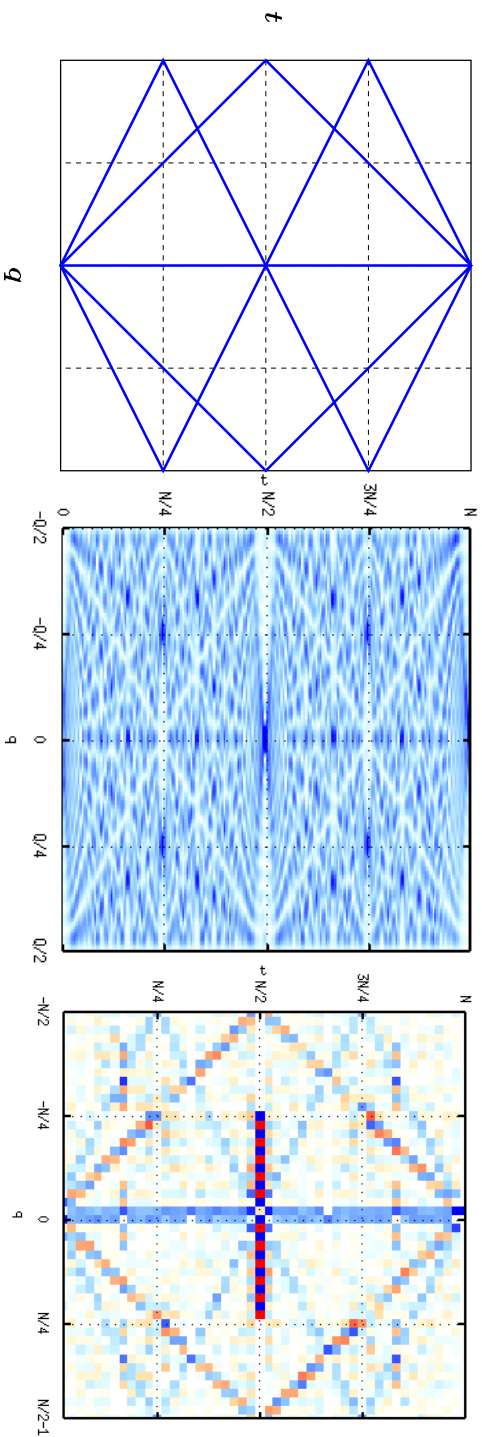
Delta spike model-Propagator



Wigner Function Propagator for $\mu = 1$, $m = 0$, $t = 0$, $N = 48$ and (a) $t' = 0$, (b) $t' = N/4$, (c)

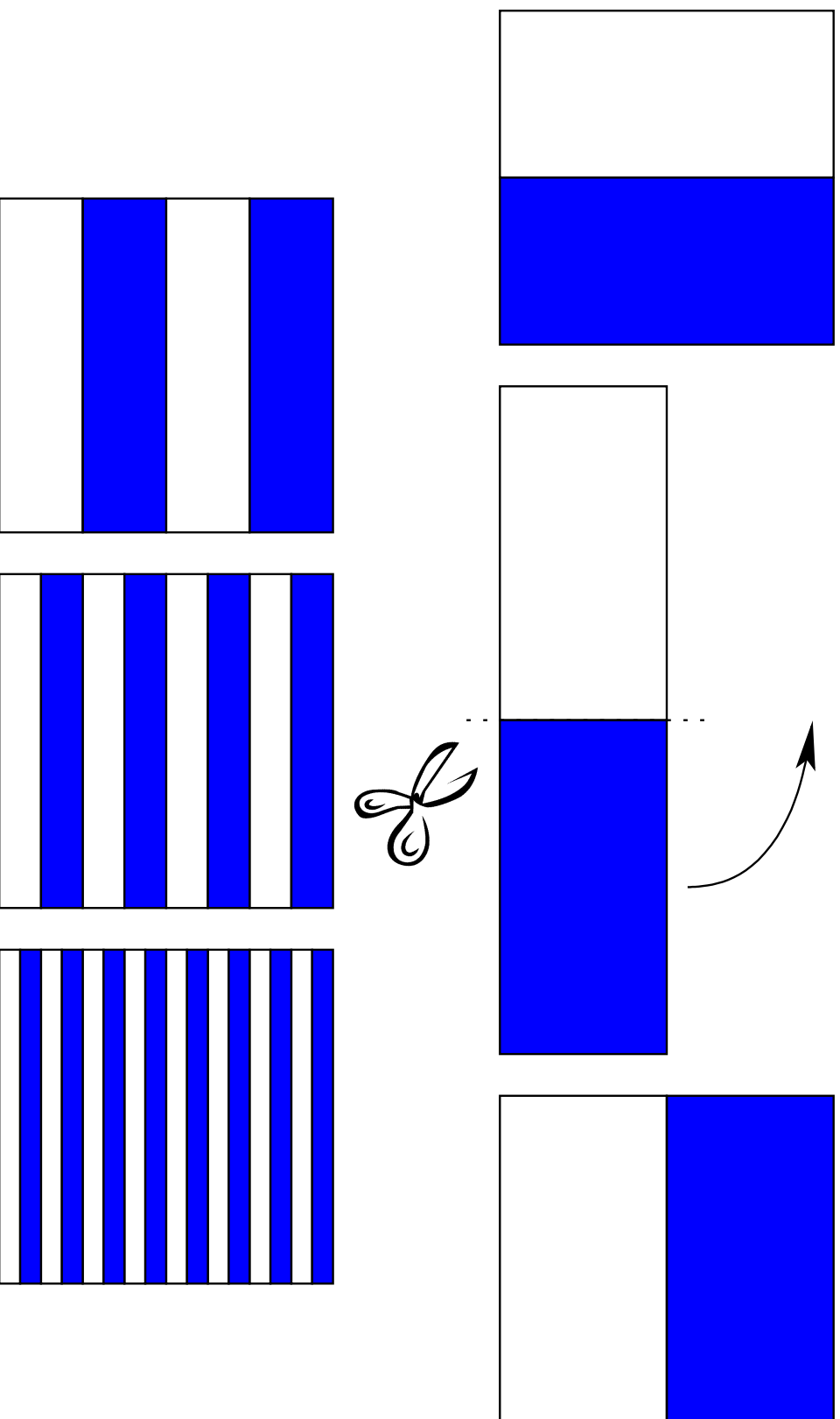
$t' = N/2$ (d) $t' = N$.

Delta Spike model - Quantum Carpets



5. Classical and quantum comparisons

Baker map



Baker map

The classical map is given by

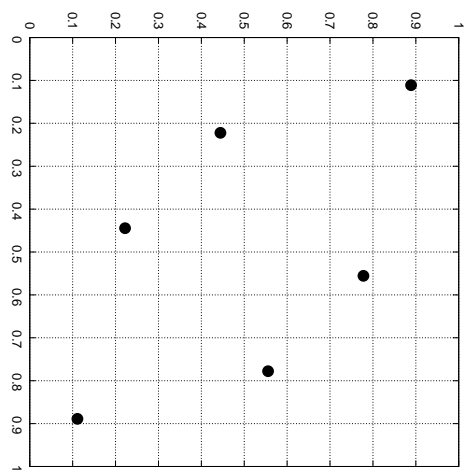
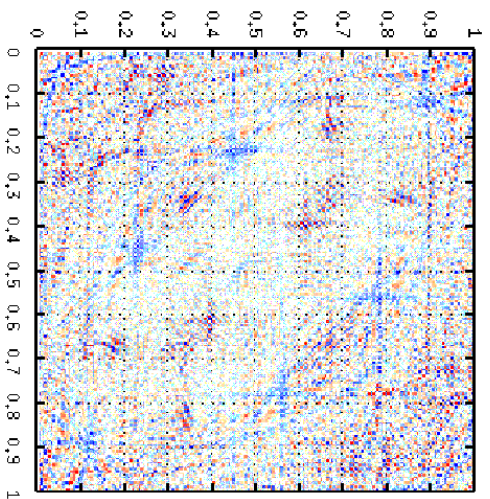
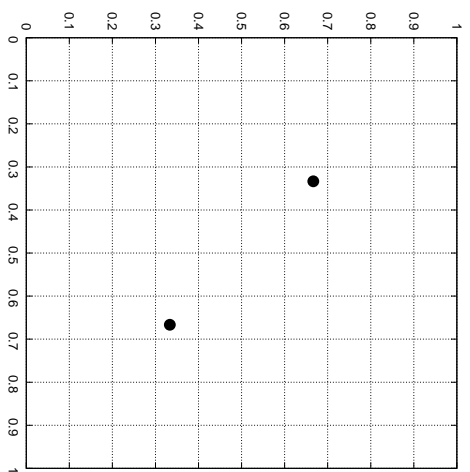
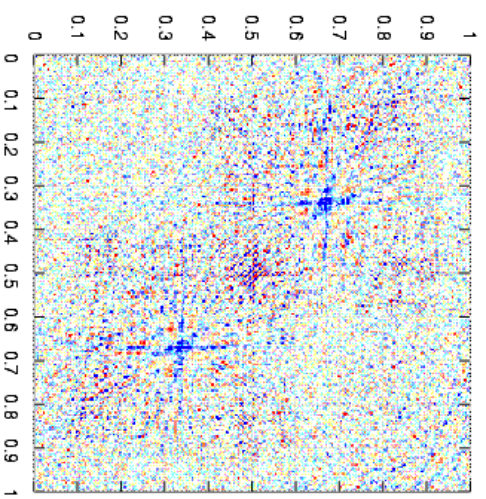
$$\begin{pmatrix} q' \\ p' \end{pmatrix} = \begin{pmatrix} 2q \\ p/2 \end{pmatrix} \quad 0 \leq q < Q/2,$$

$$\begin{pmatrix} q' \\ p' \end{pmatrix} = \begin{pmatrix} 2q - Q \\ (p + P)/2 \end{pmatrix} \quad Q/2 \leq q < Q.$$

The quantum counterpart is given by

$$\begin{pmatrix} \Psi'_R(q) \\ \Psi'_L(q) \end{pmatrix} = \mathcal{F}_N^{-1} \begin{pmatrix} \mathcal{F}_{N/2} & 0 \\ 0 & \mathcal{F}_{N/2} \end{pmatrix} \begin{pmatrix} \Psi_R(q) \\ \Psi_L(q) \end{pmatrix}.$$

Baker map



6. Conclusions

- The proposed discrete Wigner function holds with the properties of continuous version.
- Our Discrete Wigner Function allows us to define a propagator unlike the redundant definition.
- The numerical tool let us to analyze as time-independed (eigenfunctions) as time-depended (evolution) discrete systems.
- The discrete Wigner function also shows correspondence between classical and quantum mechanics.

7. Perspectives

- Analyze smooth periodic potentials like pendulum potential.
- Optimize the numerical computation to perform larger calculations.
- Analyze the relation between off-diagonal phase-space basis functions and the Ruelle-Pollicott resonances.