XXVIII. Basic Quantum Mechanics in Coordinate, Momentum & Phase Space

Tutorial: *The Wigner Quasiprobability Distribution*, Wikipedia

The Wigner quasiprobability distribution (also called the Wigner function or the Wigner–Ville distribution, after Eugene Wigner and Jean-André Ville) is a quasiprobability distribution. It was introduced by Eugene Wigner in 1932 to study quantum corrections to classical statistical mechanics. The goal was to link the wavefunction that appears in Schrödinger's equation to a probability distribution in phase space.

It is a generating function for all spatial autocorrelation functions of a given quantum-mechanical wavefunction $\psi(x)$. Thus, it maps on the quantum density matrix in the map between real phase-space functions and Hermitian operators introduced by Hermann Weyl in 1927, in a context related to representation theory in mathematics (see Weyl quantization). In effect, it is the Wigner–Weyl transform of the density matrix, so the realization of that operator in phase space.

In 1949, José Enrique Moyal, who had derived it independently, recognized it as the quantum moment-generating functional, and thus as the basis of an elegant encoding of all quantum expectation values, and hence quantum mechanics, in phase space.

Relation to classical mechanics

A classical particle has a definite position and momentum, and **hence it is represented by a point in phase space**. Given a collection (ensemble) of particles, the probability of finding a particle at a certain position in phase space is specified by a probability distribution, the Liouville density. **This strict interpretation fails for a quantum particle, due to the uncertainty principle.** Instead, the above quasiprobability Wigner distribution plays an analogous role, but does not satisfy all the properties of a conventional probability distribution; and, conversely, satisfies boundedness properties unavailable to classical distributions.

For instance, the Wigner distribution can and normally does take on negative values for states which have no classical model—and is a **convenient indicator of quantum-mechanical interference.** (See below for a characterization of pure states whose Wigner functions are non-negative.) Smoothing the Wigner distribution through a filter of size larger than ħ (e.g., convolving with a phase-space Gaussian, a Weierstrass transform, to yield the Husimi representation, below), results in a positive-semidefinite function, i.e., it may be thought to have been coarsened to a semi-classical one.

Regions of such negative value are provable (by convolving them with a small Gaussian) to be "small": they cannot extend to compact regions larger than a few ħ, and hence disappear in the classical limit. They are shielded by the uncertainty principle, which does not allow precise location within phase-space regions smaller than ħ, and thus renders such "negative probabilities" less paradoxical.

Definition and meaning

The Wigner distribution W(x,p) of a pure state is defined as

$$W(x,p) \stackrel{\text{def}}{=} \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} \psi^*(x+y)\psi(x-y)e^{2ipy/\hbar}\, dy,$$

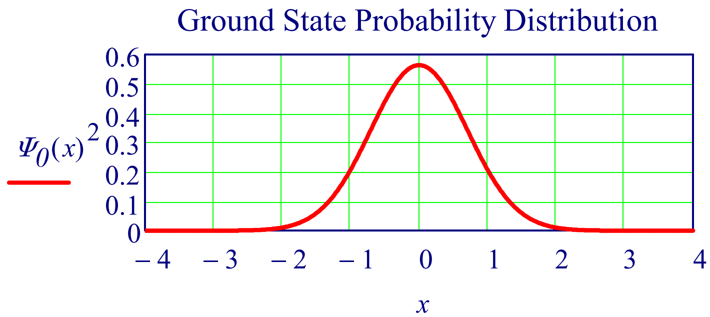
where ψ is the wavefunction, and x and p are position and momentum, but could be any conjugate variable pair (e.g. real and imaginary parts of the electric field or frequency and time of a signal). Note that it may have support in x even in regions where ψ has no support in x ("beats"). It is symmetric in x and p: See the Phase Space Distribution of the Wigner Function Expressed in Dirac Notation shown on the following page.

Ground State Probability Distribution for a Harmonic Oscillator: Math

We will use calculations on the harmonic oscillator to illustrate the relationship between the coordinate, momentum and phase space representations of quantum mechanics.
The first (ground state) oscillator eigenfunction is given below.

$$\Psi_0(x) := \pi^{\frac{-1}{4}} \cdot exp\left(\frac{-x^2}{2}\right) \qquad x := -4, -3.99 .. 4$$

As is well-known, in coordinate space the position operator is multiplicative and the momentum operator is differential. In momentum space it is the reverse, while in phase space, both position and momentum are multiplicative operators.



$$\int_{-\infty}^{\infty} \Psi_0(x)^2 dx = 1 \qquad x_{ave} = \int_{-\infty}^{\infty} x \cdot \Psi_0(x)^2 dx \rightarrow 0 \qquad x2_{ave} := \int_{-\infty}^{\infty} x^2 \cdot \Psi_0(x)^2 dx \rightarrow \frac{1}{2}$$

$$p_{ave} := \int_{-\infty}^{\infty} \Psi_0(x) \cdot \frac{1}{i} \cdot \frac{d}{dx} \Psi_0(x) dx \rightarrow 0 \qquad p2_{ave} := \int_{-\infty}^{\infty} \Psi_0(x) \cdot \frac{d^2}{dx^2} \Psi_0(x) dx \rightarrow \frac{1}{2}$$

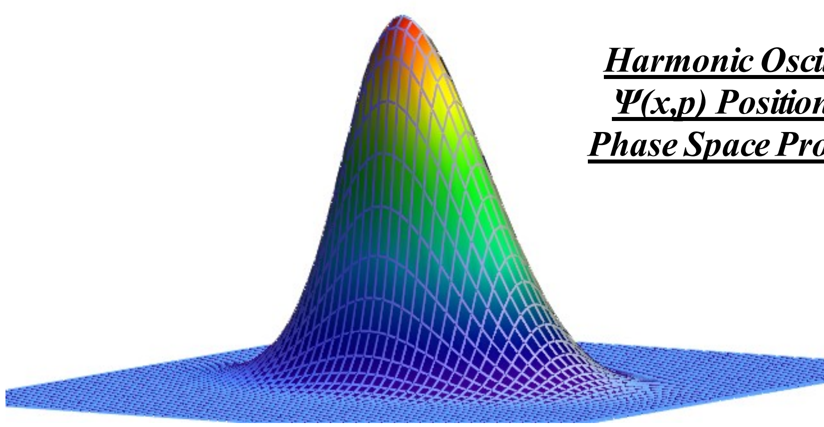
Phase Space Distribution Calculations: The Wigner Quasiprobability Distribution for a Harmonic Oscillator

Phase-space calculations require a Phase-Space Distribution, such as the Wigner function. Because this approach to quantum mechanics is not as familiar as the Schrödinger formulation, several important equations will be deconstructed using Dirac notation. **Expressed in Dirac Notation, the Wigner Function resembles a classical trajectory.**

$$W(x,p) = \int_{-\infty}^{\infty} \left\langle \Psi | x + \frac{s}{2} \right\rangle \left\langle x + \frac{s}{2} | p \right\rangle \left\langle p | x - \frac{s}{2} \right\rangle \left\langle x - \frac{s}{2} | \Psi \right\rangle ds \qquad W_0(x,p) := \frac{1}{\pi} \cdot e^{\left(-x^2\right) - p^2}$$

The four Dirac brackets are read from right to left as follows: (1) is the amplitude that a particle state Ψ has at position (x - s/2); 2 is the amplitude that a particle position (x - s/2) has momentum p; 3 is the amplitude that a particle has the momentum p has position (x +s/2); (4) is the amplitude that a particle with position (x + s/2)

$$N := 60 \qquad i := 0..N \qquad x_i := -3 + \frac{6 \cdot i}{N} \qquad j := 0..N \qquad p_j := -5 + \frac{10 \cdot j}{N} \qquad Wigner_{i,j} := W_0\left(x_i, p_j\right)$$



Harmonic Oscillator Ground State Ψ(x,p) Position - Momentum 3-D Phase Space Probability Distribution

Wigner

In these phase-space calculations W(x,p) appears to behave like a classical probability function. By eliminating the need for differential operators, it seems to have removed some of the weirdness from quantum mechanics. The Wigner function, phase-space approach only temporarily hides the weirdness generated using a Schrödinger wave function.

To see how the weirdness is hidden we generate the Wigner function for the v = 2 harmonic oscillator state.

$$W_1(x,p) := \frac{1}{2\pi}\int_{-\infty}^{\infty} \Psi_1\left(x+\frac{s}{2}\right)\cdot \exp(i\cdot s\cdot p)\cdot \Psi_1\left(x-\frac{s}{2}\right) ds \text{ simplify}$$

$$W_1(x,p) := e^{-\left(x^2\right)-p^2}\cdot\frac{\left(2\cdot x^2+2\cdot p^2\right)-1}{\pi}$$

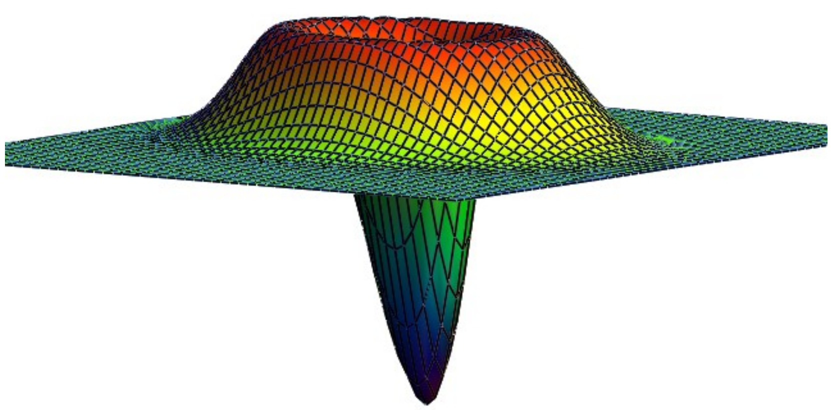
Next, it is demonstrate that the Wigner functions for the ground and excited harmonic oscillator states are orthogonal over phase space.

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} W_0(x,p)\cdot W_1(x,p)dxdp \rightarrow 0$$

This result indicates that W1(x,p) must be negative over some part of phase space, because the graph of W0(x,p) shows that it is positive for all values of position and momentum. To explore further we display the Wigner distribution for the v = 1 harmonic oscillator state.

$$Wigner_{i,j} := W_1\left(x_i, p_j\right)$$

Harmonic Oscillator v = 1 State
Ψ(x,p) Position - Momentum 3-D Phase Space
Probability Distribution



Wigner , Wigner

Given the quantum number this Mathcad file calculates the Wigner distribution function for the specified harmonic oscillator eigen state.

Quantum number: n:=2

Harmonic oscillator eigenstate:

$$n := 2 \qquad \Psi_2(x) := \frac{1}{\sqrt{2^n \cdot n! \cdot \sqrt{\pi}}} \cdot Her(n,x) \cdot exp\left(\frac{-x^2}{2}\right)$$

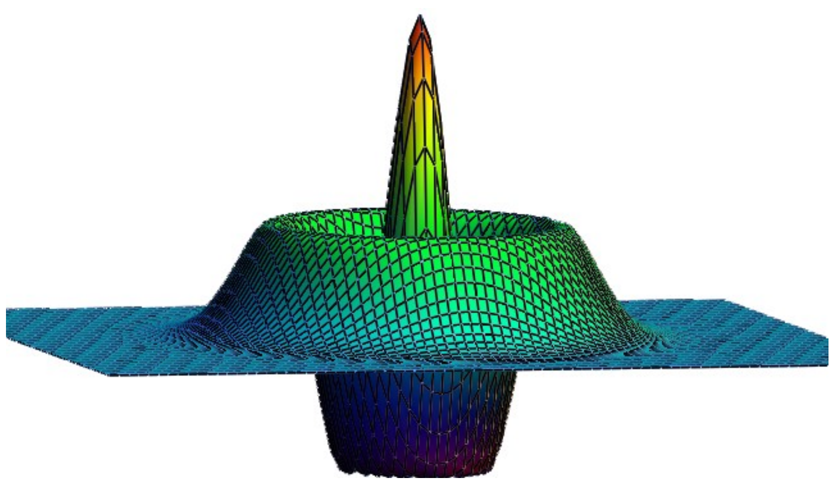
Calculate the Wigner distribution:

$$W_{n2}(x,p) := \frac{1}{\pi^{\frac{3}{2}}} \cdot \int_{-\infty}^{\infty} \Psi_2\left(x+\frac{s}{2}\right) \cdot exp(i \cdot s \cdot p) \cdot \Psi_2\left(x-\frac{s}{2}\right) ds$$

Display the Wigner distribution:

$$N := 80 \qquad i := 0..N \qquad x_i := -4 + \frac{8 \cdot i}{N} \qquad j := 0..N \qquad p_j := -5 + \frac{10 \cdot j}{N} \qquad Wigner2_{i,j} := W_{n2}(x_i, p_j)$$

Harmonic Oscillator v = 2 State
Ψ(x,p) Position - Momentum 3-D Phase Space
Probability Distribution



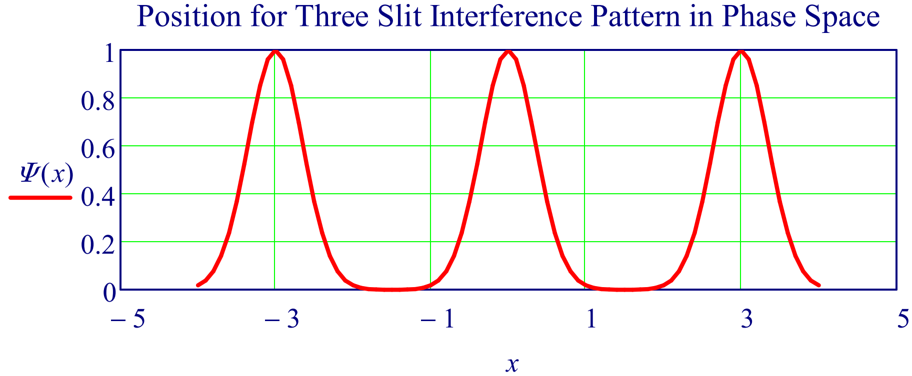
$Wigner2, Wigner2$

Basic QM Math: Wigner Quasiprobability Distribution for Triple-Slit Experiment

The quantum mechanical interpretation of the triple-slit experiment is that position is measured at the slit screen and momentum is measured at the detection screen. Position and momentum are conjugate observables connected by a Fourier transform and governed by the uncertainty principle. Knowing the slit screen geometry makes it possible to calculate the momentum distribution at the detection screen.

The slit-screen geometry and therefore the coordinate wavefunction is modeled as a superposition of three Gaussian functions.

$$\Psi(x) := exp\left[-4\cdot(x-3)^2\right] + exp\left(-4\cdot x^2\right) + exp\left[-4\cdot(x+3)^2\right]$$



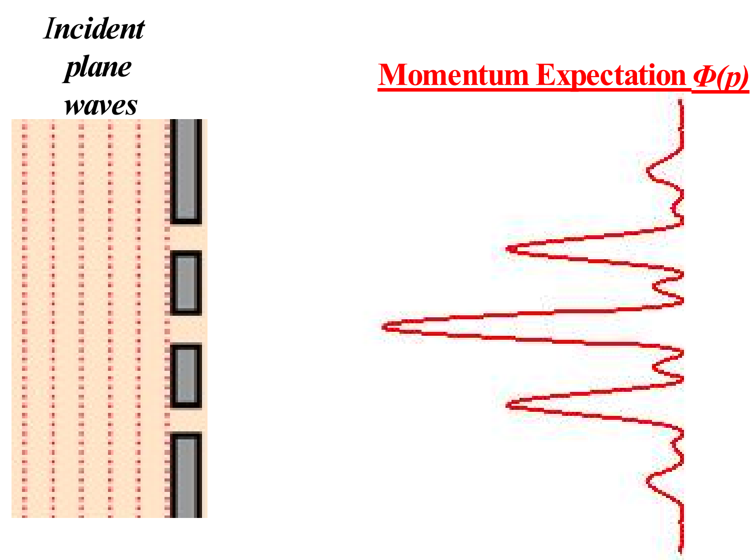
The coordinate wavefunction is Fourier transformed into momentum space to yield the diffraction pattern. Note that this calculation is in agreement with the expectation that the number of minor maxima appearing between the major maxima is given by the number of slits minus 2.

Momentum Expectation Function

$$\Phi(p) := \frac{1}{\sqrt{2\pi}}\cdot\int_{-\infty}^{\infty} exp(-i\cdot p\cdot x)\cdot \Psi(x)\, dx$$

$$p := -6, -5.95 .. 6$$

Three Slit Demonstration for Momentum *Φ(p)*

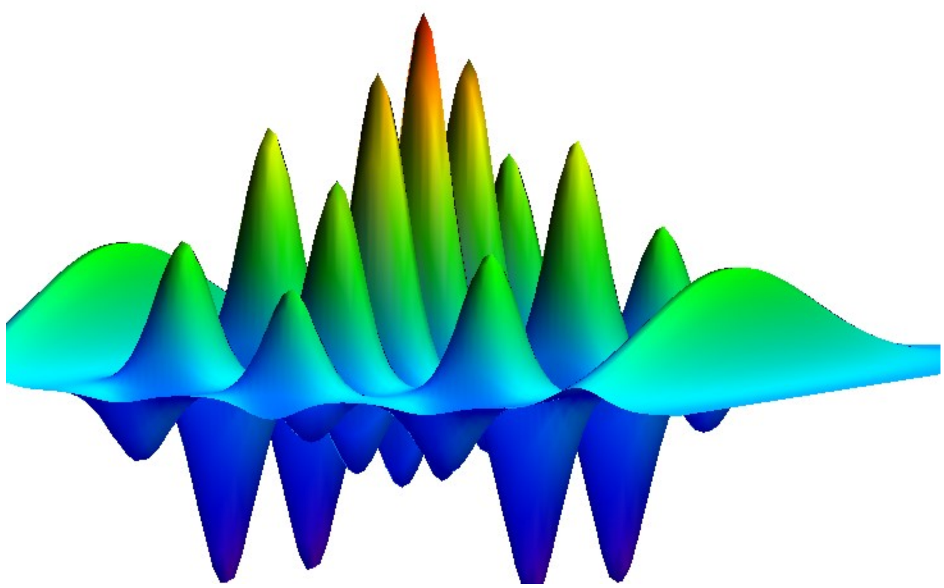


The Wigner function is a phase-space distribution that is obtained by the Fourier transform of either the coordinate or momentum wavefunction. We use the coordinate wavefunction.

$$W(x,p) := \frac{1}{\pi^{\frac{3}{2}}} \cdot \int_{-20}^{20} \Psi\left(x + \frac{s}{2}\right) \cdot exp(-i \cdot s \cdot p) \cdot \Psi\left(x - \frac{s}{2}\right) ds$$

$N := 100 \qquad i := 0..N \qquad x_i := -4 + \frac{8 \cdot i}{N}$

$j := 0..N \qquad p_j := -6 + \frac{12 \cdot j}{N} \qquad Wigner_{3\phi_{i,j}} := W\left(x_i, p_j\right)$



$Wigner_{3\phi}$

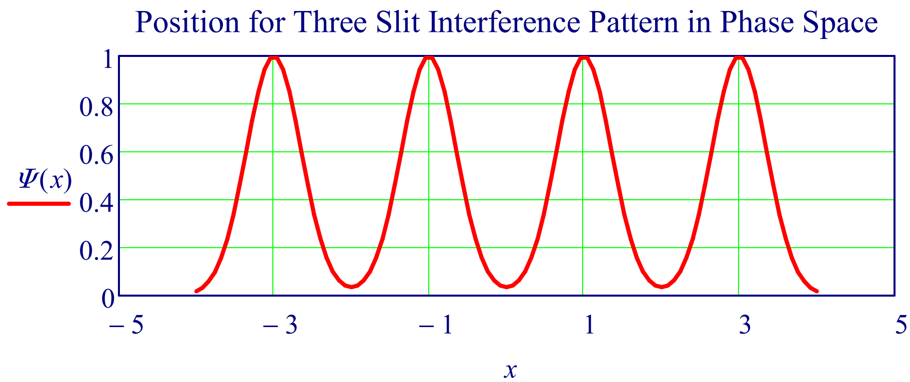
The Wigner distribution is frequently called a quasi-probability distribution because, as can be seen in the display above, it can have negative values. Integration of the Wigner function with respect to momentum recovers the coordinate wavefunction and integration with respect to position yields the momentum wavefunction.

Basic QM: Wigner Quasiprobability Distribution: Quadruple-Slit Experiment

The quantum mechanical interpretation of the triple-slit experiment is that position is measured at the slit screen and momentum is measured at the detection screen. Position and momentum are conjugate observables connected by a Fourier transform and governed by the uncertainty principle. Knowing the slit screen geometry makes it possible to calculate the momentum distribution at the detection screen.

The slit-screen geometry and therefore the coordinate wavefunction is modeled as a superposition of three Gaussian functions.

$$\Psi(x) := exp\left[-4\cdot(x-3)^2\right] + exp\left[-4\cdot(x-1)^2\right] + exp\left[-4\cdot(x+1)^2\right] + exp\left[-4\cdot(x+3)^2\right]$$

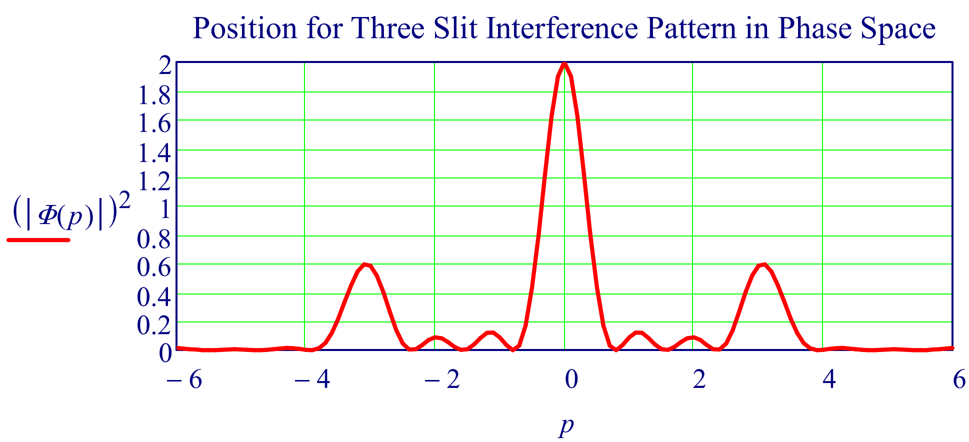


The coordinate wavefunction is Fourier transformed into momentum space to yield the diffraction pattern. Note that this calculation is in agreement with the expectation that the number of minor maxima appearing between the major maxima is given by the number of slits minus 2.

Momentum Expectation Function

$$\Phi(p) := \frac{1}{\sqrt{2\pi}} \cdot \int_{-6}^{6} exp(-i \cdot p \cdot x) \cdot \Psi(x)\, dx$$

$$p := -6, -5.9 .. 6$$

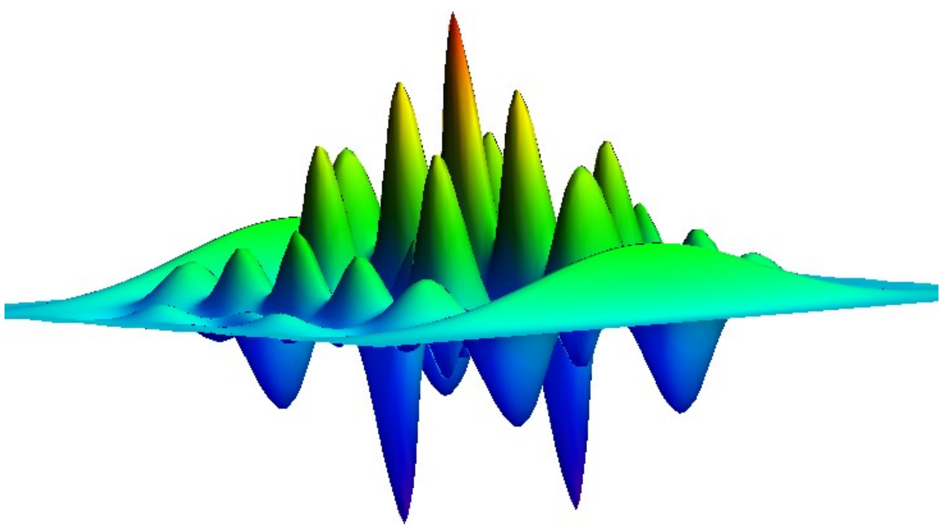


The coordinate wavefunction is Fourier transformed into momentum space to yield the diffraction pattern. Note that this calculation is in agreement with the expectation that the number of minor maxima appearing between the major maxima is given by the number of slits minus 2.

$$W(x,p) := \frac{1}{\pi^{\frac{3}{2}}} \cdot \int_{-20}^{20} \Psi\left(x + \frac{s}{2}\right) \cdot exp(i \cdot s \cdot p) \cdot \Psi\left(x - \frac{s}{2}\right) ds$$

$N := 100 \qquad i := 0..N \qquad x_i := -4 + \frac{8 \cdot i}{N}$

$j := 0..N \qquad p_j := -6 + \frac{12 \cdot j}{N} \qquad Wigner_{4\phi_{i,j}} := W\left(x_i, p_j\right)$



$Wigner_{4\phi}$