The WKB approximation in deformation quantization

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Jaromir Tosiek

Lodz University of Technology, Poland

in collaboration with

Ruben Cordero and **Francisco Turrubiates**

Instituto Politecnico Nacional, Mexico

1 The energy $*$– eigenvalue equation

For a Hamilton function $H(\vec{r},\vec{p}) = \frac{\vec{p}^2}{2M} + V(\vec{r})$ the $*$– eigenvalue equation is

$$H(\vec{r},\vec{p}) * W_E(\vec{r},\vec{p}) = E\, W_E(\vec{r},\vec{p})$$

with an additional condition imposed on the Wigner energy eigenfunction $W_E(\vec{r},\vec{p})$

$$\{H(\vec{r},\vec{p}), W_E(\vec{r},\vec{p})\}_{\mathrm{M}} = 0.$$

As the ∗− product we use the Moyal product

$$A(\vec{r},\vec{p}) * B(\vec{r},\vec{p}) := \frac{1}{(\pi\hbar)^6}\int_{\mathbb{R}^{12}} d\vec{r}\,'d\vec{p}\,'d\vec{r}\,''d\vec{p}\,''A(\vec{r}\,',\vec{p}\,')B(\vec{r}\,'',\vec{p}\,'')$$

$$\times \exp\left[\frac{2i}{\hbar}\Big\{(\vec{r}\,''-\vec{r})\cdot(\vec{p}\,'-\vec{p})-(\vec{r}\,'-\vec{r})\cdot(\vec{p}\,''-\vec{p})\Big\}\right].$$

The dot '·' stands for the scalar product.

The above definition is valid for a wide class of tempered distributions.

The Moyal product is closed i.e.

$$\int_{\mathbb{R}^6} A(\vec{r},\vec{p}) * B(\vec{r},\vec{p}) d\vec{r}\, d\vec{p} = \int_{\mathbb{R}^6} B(\vec{r},\vec{p}) * A(\vec{r},\vec{p}) d\vec{r}\, d\vec{p} =$$

$$\int_{\mathbb{R}^6} A(\vec{r},\vec{p}) \cdot B(\vec{r},\vec{p}) d\vec{r}\, d\vec{p}.$$

The mean value of a function $A(\vec{r},\vec{p})$ in a state represented by a Wigner function $W(\vec{r},\vec{p})$ equals

$$\Big\langle A(\vec{r},\vec{p}) \Big\rangle = \int_{\mathbb{R}^6} A(\vec{r},\vec{p}) \cdot W(\vec{r},\vec{p}) d\vec{r}\, d\vec{p}.$$

The Moyal bracket is defined as

$$\{A(\vec{r},\vec{p}),B(\vec{r},\vec{p})\}_{\mathrm{M}} := \frac{1}{i\hbar}\Big(A(\vec{r},\vec{p})*B(\vec{r},\vec{p}) - B(\vec{r},\vec{p})*A(\vec{r},\vec{p})\Big).$$

Not all of the solutions of the system of the $*$- eigenvalue equations are physically acceptable.

A Wigner eigenfunction $W_E(\vec{r},\vec{p})$ of the Hamilton function $H(\vec{r},\vec{p})$ fulfills the following conditions:

(i) is a real function,

(ii) the $*-$ square $W_E(\vec{r},\vec{p}) * W_E(\vec{r},\vec{p}) = \frac{1}{2\pi\hbar} W_E(\vec{r},\vec{p})$ and

(iii) $\int_{\mathbb{R}^6} W_E(\vec{r},\vec{p}) d\vec{r} d\vec{p} = 1.$

We restrict to the 1– D case. But even in this simplest situation the system of eigenvalue equations leads to a pair of integral equation. This is why approximate methods are desirable.

A naive treating of the $*$ – eigenvalue equation as a power series in the deformation parameter $\hbar$ does not work, because Wigner eigenfunctions contain arbitrary large negative powers of $\hbar$.

2 Ingredients of the WKB construction

Eigenstates and eigenvalues of energy can be found by solving the stationary Schroedinger equation

$$-\frac{\hbar^2}{2M}\Delta\psi_E(\vec{r}) + V(\vec{r})\psi_E(\vec{r}) = E\psi_E(\vec{r}).$$

Every solution of the stationary Schroedinger equation can be written as a linear combination of two functions

$$\psi_{E\,I}(\vec{r}) = \exp\left(\frac{i}{\hbar}\sigma_I(\vec{r})\right) \quad \text{and} \quad \psi_{E\,II}(\vec{r}) = \exp\left(\frac{i}{\hbar}\sigma_{II}(\vec{r})\right),$$

where $\sigma_I(\vec{r}), \sigma_{II}(\vec{r})$ denote some complex valued functions.

When we substitute functions $\psi_{E\,I}(\vec{r}\,), \psi_{E\,II}(\vec{r}\,)$ into the stationary Schroedinger equation, we obtain that phases $\sigma_I(\vec{r}\,)$ and $\sigma_{II}(\vec{r}\,)$ satisfy the partial nonlinear differential equation of the 2nd order

$$\frac{1}{2M}\big(\nabla\sigma(\vec{r}\,)\big)^2 - \frac{i\hbar}{2M}\Delta\sigma(\vec{r}\,) = E - V(\vec{r}), \qquad (1)$$

for $\sigma(\vec{r}\,) = \sigma_I(\vec{r}\,)$ and $\sigma(\vec{r}\,) = \sigma_{II}(\vec{r}\,)$.

In the classical limit $\hbar \to 0$ this equation reduces to the Hamilton – Jacobi stationary equation

$$\frac{1}{2M}\big(\nabla\sigma(\vec{r}\,)\big)^2 = E - V(\vec{r}). \qquad (2)$$

In the 1–D case Eq. (1) is of the form

$$\frac{1}{2M}\left(\frac{d\sigma(x)}{dx}\right)^2 - \frac{i\hbar}{2M}\frac{d^2\sigma(x)}{dx^2} = E - V(x).$$

In some part of its domain the solution can be written as a formal power series in the Planck constant

$$\sigma(x) = \sum_{k=0}^{\infty}\left(\frac{\hbar}{i}\right)^k \sigma_k(x).$$

Thus we receive an iterative system of equations

$$
\begin{aligned}
\frac{1}{2M}\left(\frac{d\sigma_0(x)}{dx}\right)^2 &= E - V(x), \\
\frac{d\sigma_0(x)}{dx}\frac{d\sigma_1(x)}{dx} + \frac{1}{2}\frac{d^2\sigma_0(x)}{dx^2} &= 0, \\
\frac{d\sigma_0(x)}{dx}\frac{d\sigma_2(x)}{dx} + \frac{1}{2}\left(\frac{d\sigma_1(x)}{dx}\right)^2 + \frac{1}{2}\frac{d^2\sigma_1(x)}{dx^2} &= 0, \\
\vdots \quad \vdots \quad &\vdots
\end{aligned}
$$

There are two solutions of these equations. They differ on the sign at even $\hbar$ power elements.

In the case when the phase $\sigma(x)$ is the power series in the Planck constant, the wave function

$$\psi_E(x) = \prod_{k=0}^{\infty} \psi_{E\,k}(x) \quad , \quad \psi_{E\,k}(x) = \exp\left[\frac{i}{\hbar}\left(\frac{\hbar}{i}\right)^k \sigma_k(x)\right] .$$

Each function $\psi_{E\,k}(x)$ need not be an element of $L^2(\mathbb{R})$ but as it is smooth and, due to physical requirements, bounded, the product $\overline{\psi}_{E\,k}\left(x + \frac{\xi}{2}\right)\psi_{E\,k}\left(x - \frac{\xi}{2}\right)$ is a tempered generalised function.

The analysed approximation can be realised as an iterative procedure, in which the n-th approximation $\psi_{E(n)}(x)$ of the wave function $\psi_E(x)$ equals

$$\psi_{E(0)}(x) := \psi_{E0}(x)$$

$$\psi_{E(n)}(x) = \psi_{E(n-1)}(x) \cdot \psi_{E\,n}(x)\ ,\ n \geqslant 1.$$

Applying the Weyl correspondence $\mathbf{W}^{-1}$ to an energy eigenstate $\psi_E(x) := \langle x|\psi_E\rangle = \exp\left(\frac{i}{\hbar}\sigma(x)\right)$ we see that its Wigner function is of the form

$$W_E(x,p) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} d\xi\, \overline{\psi}_E\left(x+\frac{\xi}{2}\right)\psi_E\left(x-\frac{\xi}{2}\right)\exp\left(-\frac{i\xi p}{\hbar}\right) =$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} d\xi\, \exp\left(\frac{i}{\hbar}\left[\sigma\left(x-\frac{\xi}{2}\right)-\overline{\sigma}\left(x+\frac{\xi}{2}\right)-\xi p\right]\right).$$

Thus

$$W_{E(n)}(x,p) = \int_{-\infty}^{+\infty} W_{E(n-1)}(x,p')W_{E\,n}(x,p-p')dp' =$$

$$= \int_{-\infty}^{+\infty} W_{E(n-1)}(x,p-p'')W_{E\,n}(x,p'')dp''.$$

The semiclassical approximation cannot be applied everywhere. Thus the wave function is a sum of spatially separable functions

$$\psi_E(x) = \sum_{l=1}^{k} \psi_{Ea_l b_l}(x)$$
$$-\infty \leqslant a_1 < b_1 = a_2 < b_2 = a_3 < \ldots < b_{k-1} = a_k < b_k \leqslant \infty.$$

It is a vital question about a phase space counterpart of a state being the superposition of wave functions.

Let us consider a Wigner function originating from a wave function $\psi_{Ea_lb_l}(x)$.

$$W_{Ea_lb_l}(x,p) = \frac{1}{2\pi\hbar}\int_{\mathrm{Max.}[2(a_l-x),2(x-b_l)]}^{\mathrm{Min.}[2(x-a_l),2(b_l-x)]} d\xi\, \overline{\psi}_{Ea_lb_l}\left(x+\frac{\xi}{2}\right)\times$$
$$\times\psi_{Ea_lb_l}\left(x-\frac{\xi}{2}\right)\exp\left(-\frac{i\xi p}{\hbar}\right).$$

(i) The Wigner function $W_{Ea_lb_l}(x,p)$ vanishes outside the set $(a_l,b_l)\times\mathbb{R}$.

(ii) As the function $\psi_{Ea_lb_l}(x)$ itself can be a sum of functions, we see that every Wigner function of a superposition of wave functions with supports from an interval $[a_l,b_l]$ is still limited to the strip $a_l\leqslant x\leqslant b_l$.

One can deduce that if an operator $\hat{A}$ in the position representation satisfies the condition

$$\langle x|\hat{A}|x'\rangle \neq 0 \quad \text{only} \;\; \text{for} \quad a < x, x' < b,$$

then the function $\mathbf{W}^{-1}(\hat{A})(x,p)$ may be different from 0 only for x contained in the interval (a,b). Moreover, the function $\mathbf{W}^{-1}(\hat{A})(x,p)$ is a smooth function respect to the momentum p. For every $\tilde{x} \in (a,b)$ and every positive number $\Lambda > 0$ there exists a value of momentum $\tilde{p}$ such that $|\tilde{p}| > \Lambda$ and $\mathbf{W}^{-1}(\hat{A})(\tilde{x},\tilde{p}) \neq 0$.

Consider a two-component linear combination of functions

$$Y(x-a_l)\psi_{Ea_lb_l}(x)Y(b_l-x)+Y(x-a_r)\psi_{Ea_rb_r}(x)Y(b_r-x),$$

$$-\infty\leqslant a_l<b_l\leqslant a_r<b_r\leqslant\infty.$$

Its Wigner function

$$W_E(x,p)=\mathbf{W}^{-1}\Big(\frac{1}{2\pi\hbar}|\psi_{Ea_lb_l}\rangle\langle\psi_{Ea_lb_l}|\Big)+\mathbf{W}^{-1}\Big(\frac{1}{2\pi\hbar}|\psi_{Ea_rb_r}\rangle\langle\psi_{Ea_rb_r}|\Big)+$$

$$+\mathbf{W}^{-1}\Big(\frac{1}{2\pi\hbar}|\psi_{Ea_lb_l}\rangle\langle\psi_{Ea_rb_r}|+\frac{1}{2\pi\hbar}|\psi_{Ea_rb_r}\rangle\langle\psi_{Ea_lb_l}|\Big).$$

The interference operator $\hat{\text{Int}} := |\psi_{Ea_lb_l}\rangle\langle\psi_{Ea_rb_r}| + |\psi_{Ea_rb_r}\rangle\langle\psi_{Ea_lb_l}|$

(i) is self-adjoint.

(ii) It is not a projector.

(iii) Its trace vanishes and it has three possible eigenvalues λ:

$$\lambda = -||\psi_{Ea_lb_l}||\cdot||\psi_{Ea_rb_r}||, |-\rangle = \frac{1}{\sqrt{2}}\left(\frac{1}{||\psi_{Ea_lb_l}||}|\psi_{Ea_lb_l}\rangle - \frac{1}{||\psi_{Ea_rb_r}||}|\psi_{Ea_rb_r}\rangle\right)$$

$$\lambda = 0\ ,\ \text{its eigenvector is every vector orthogonal to } |\psi_{Ea_lb_l}\rangle \text{ and } |\psi_{Ea_rb_r}\rangle,$$

$$\lambda = ||\psi_{Ea_lb_l}||\cdot||\psi_{Ea_rb_r}||, |+\rangle = \frac{1}{\sqrt{2}}\left(\frac{1}{||\psi_{Ea_lb_l}||}|\psi_{Ea_lb_l}\rangle + \frac{1}{||\psi_{Ea_rb_r}||}|\psi_{Ea_rb_r}\rangle\right).$$

The interference operator $\hat{\mathrm{Int}}$ exchanges directions of vectors $|\psi_{Ea_lb_l}\rangle \rightleftharpoons |\psi_{Ea_rb_r}\rangle$.

$$\hat{\mathrm{Int}}|\psi_{Ea_lb_l}\rangle = ||\psi_{Ea_lb_l}||^2\,|\psi_{Ea_rb_r}\rangle \quad , \quad \hat{\mathrm{Int}}|\psi_{Ea_rb_r}\rangle = ||\psi_{Ea_rb_r}||^2\,|\psi_{Ea_lb_l}\rangle.$$

The function $W_{E\,int}(x,p)$ representing the interference term is determined by the integral

$$W_{E\,int}(x,p) = 2\Re\left(\int_{\mathrm{Max.}[2(a_l-x),2(x-b_r)]}^{\mathrm{Min.}[2(b_l-x),2(x-a_r)]} d\xi\,\overline{\psi}_{Ea_lb_l}\left(x+\frac{\xi}{2}\right)\psi_{Ea_rb_r}\left(x-\frac{\xi}{2}\right)\times \right.$$
$$\left.\times\exp\left(-\frac{i\xi p}{\hbar}\right)\right).$$

The function $W_{E\,int}(x,p)$

(i) is different from 0 for $x \in \left(\frac{a_l+a_r}{2}, \frac{b_l+b_r}{2}\right)$. This interval in general is not contained in the sum of intervals $(a_l, b_l) \cup (a_r, b_r)$.

(ii) Hence the interference part of a Wigner function may be nonzero at points with abscissas, at which two wave functions $\psi_{Ea_lb_l}(x)$ and $\psi_{Ea_rb_r}(x)$ disappear.

(iii) The function $W_{E\,int}(x,p)$ is real.

(iv) It does not contribute to the spatial density of probability, because

$$\varrho_{int}(x) = \int_{-\infty}^{+\infty} dp\, W_{E\,int}(x,p) = 0.$$

(v) Hence

$$\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dp\, W_{E\,int}(x,p) = \int_{\frac{a_l+a_r}{2}}^{\frac{b_l+b_r}{2}} dx \int_{-\infty}^{+\infty} dp\, W_{E\,int}(x,p) = 0.$$

(vi) The integrals

$$\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dp\, W_{E\,int}(x,p) W_{Ea_lb_l}(x,p) = 0,$$
$$\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dp\, W_{E\,int}(x,p) W_{Ea_rb_r}(x,p) = 0$$

vanish.

(vii) For any observable $A(x)$ depending only on position, the interference Wigner function $W_{E\,int}(x,p)$ does not influence the mean value of $A(x)$, because

$$\Big\langle A(x) \Big\rangle = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dp\, W_{E\,int}(x,p) A(x) = 0.$$

The ground state of a 1–D harmonic oscillator is

$$\psi_E(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right) \quad , \quad E = \frac{\hbar\omega}{2}.$$

It can be written as

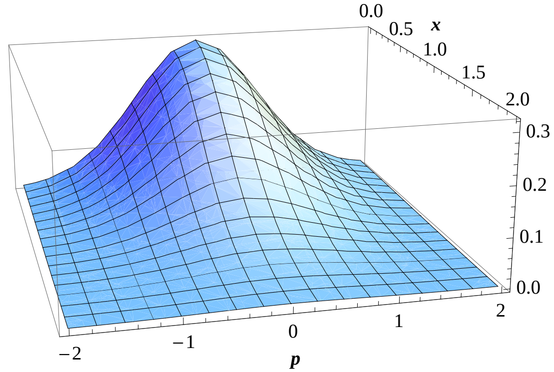
$$\psi_E(x) = \psi_{E(-)}(x) + \psi_{E(+)}(x),$$

where

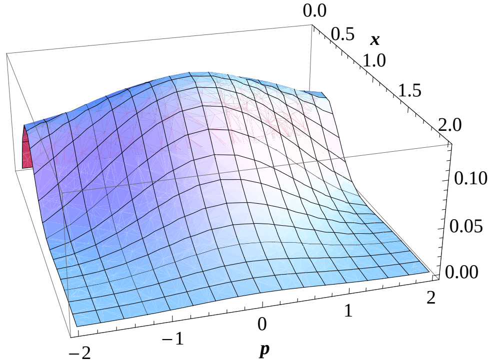
$$\psi_{E(-)}(x) = \psi_E(x)Y(-x) \quad , \quad \psi_{E(+)}(x) = \psi_E(x)Y(x).$$

Its Wigner eigenfunction

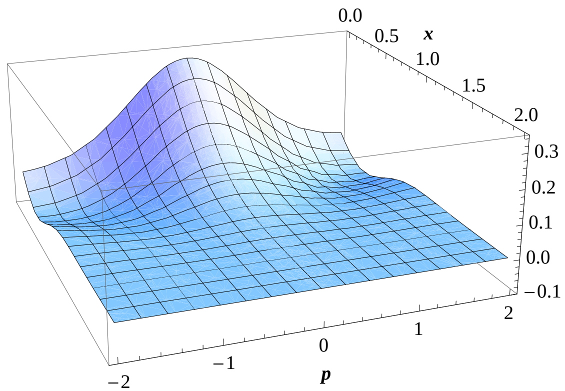
$$W_E(x,p) = \frac{1}{\pi\hbar} \exp\left(-\frac{p^2 + m^2\omega^2x^2}{\hbar m\omega}\right).$$



(a) The complete Wigner eigenfunction



(b) The Wigner energy eigenfunction without the interference contribution



(c) The interference Wigner eigenfunction

3 The WKB construction on a phase space

(i) Division of a spatial domain into parts, in which the approximation can be applied and areas near to turning points.

(ii) Approximate (up to a chosen degree) and strict solving of respective equations for the phase σ in all regions.

(iii) Application of connection formulas - finding approximate energy levels.

(iv) Calculating Wigner energy eigenfunctions.

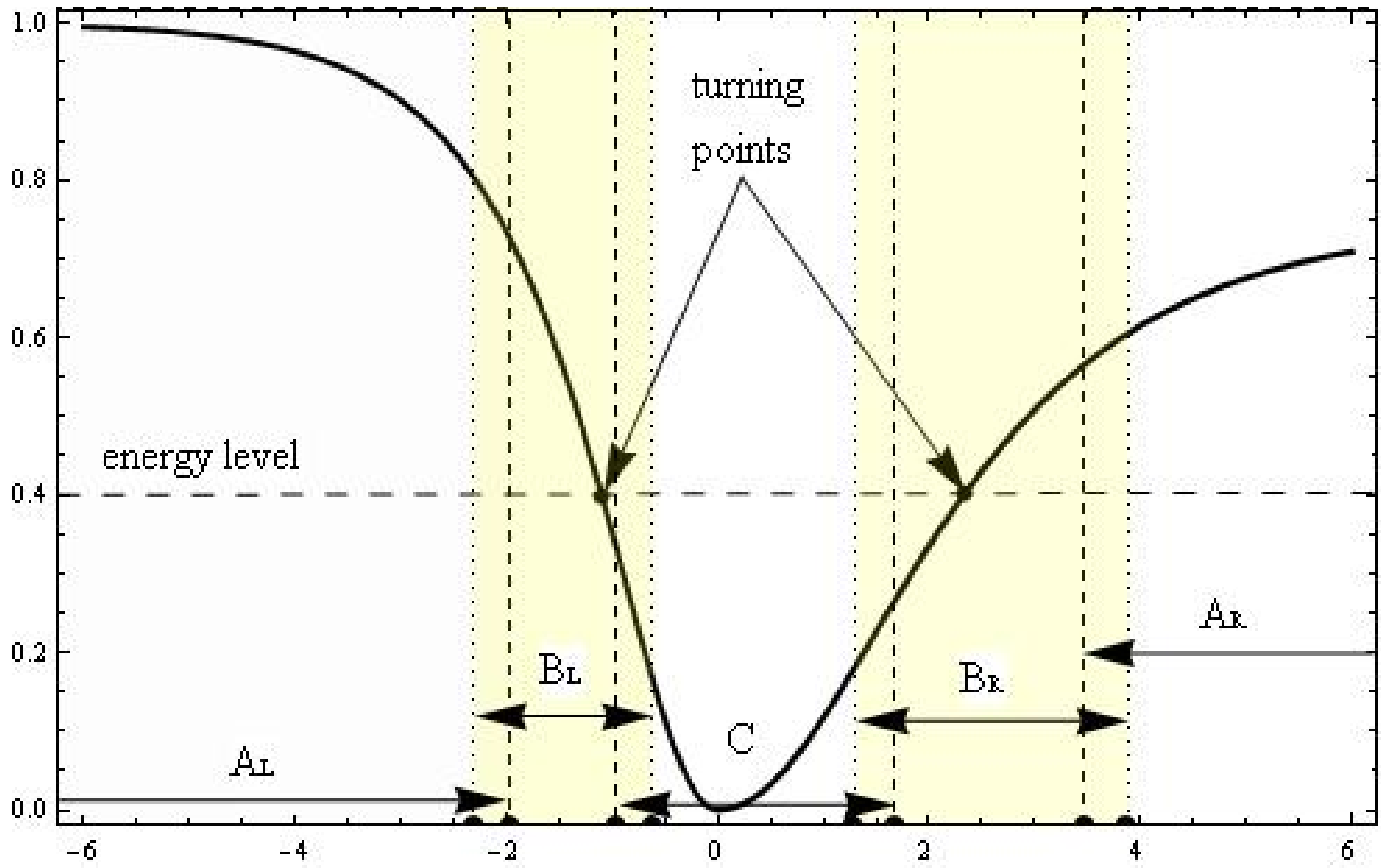


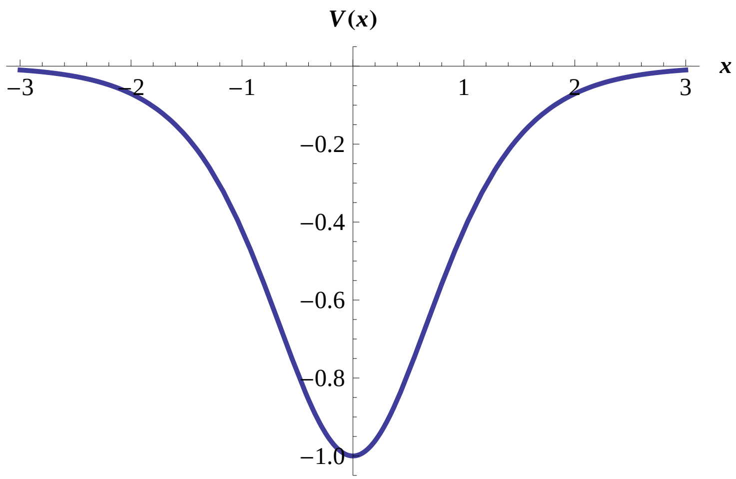
Figure 1: A potential $V(x)$ as a function of x.

4 Example

The Poeschl – Teller potential described by the expression

$$V(x) = -\frac{\hbar^2 a^2}{M} \frac{1}{\cosh^2(ax)},$$

where $a > 0$ is a parameter.



The energy eigenvalue problem for this potential is solvable for any positive energy $E > 0$

The phases

$$\sigma_0 = \frac{\hbar\sqrt{k^2\cosh^2 ax + 2a^2}}{\sqrt{k^2\cosh 2ax + 4a^2 + k^2}}\left[2\arctan\left(\frac{2a\sinh ax}{\sqrt{k^2\cosh 2ax + 4a^2 + k^2}}\right) + \frac{k}{a}\text{arcsinh}\left(\frac{k\sinh ax}{\sqrt{2a^2 + k^2}}\right)\right]$$

and

$$\sigma_1 = -\frac{1}{2}\ln\left(\hbar\cosh ax\sqrt{k^2\cosh^2 ax + 2a^2}\right).$$

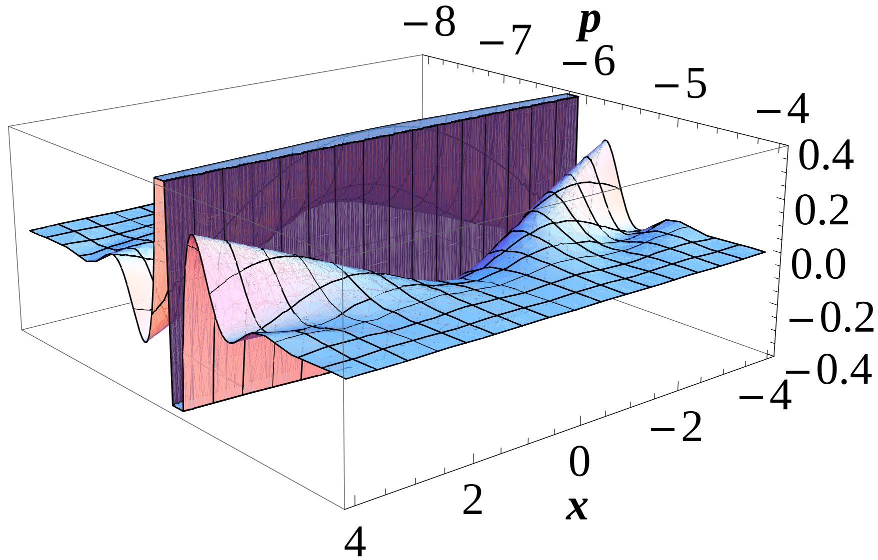


Figure 2: The strict Wigner function of the Poeschl – Teller potential.