Semiclassical Double-Inequality on Heisenberg Uncertainty Relation in 1D

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We prove a double-inequality for the product of uncertainties for position and momentum of bound states for 1D quantum mechanical systems in the semiclassical limit.

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1. Introduction

It is known that the product of position and momentum uncertainties for the N-th bound states of (i) the harmonic oscillator and (ii) the infinite square well is exactly given as

$$\frac{\Delta x \Delta p}{\hbar} = N + \frac{1}{2}, \quad N \in \mathbb{N}_0, \tag{1.1}$$

and

$$\frac{\Delta x \Delta p}{\hbar} = \frac{1}{2}\sqrt{\frac{(\pi N)^2}{3} - 2}, \quad N \in \mathbb{N}, \tag{1.2}$$

respectively. In particular, they display a linear dependence of N for $N \gg 1$. The asymptotic slope $\frac{\pi}{2\sqrt{3}} \approx 0.9069$ of the infinite square well (1.2) is less than 10% smaller than the corresponding slope (=1) of the harmonic oscillator (1.1). It is natural to ponder if there (for quantum mechanical systems in 1D) exists a semiclassical double-inequality of the form

$$C_{\min} \leq U := \frac{\Delta x \Delta p}{\hbar N} \leq C_{\max} \quad \text{for} \quad N \gg 1, \tag{1.3}$$

where $C_{\max} > C_{\min} > 0$ are two dimensionless constants, say, of order one? (The upper bound $C_{\max}$ cannot be much smaller than one in order not to conflict with the theoretical Heisenberg uncertainty bound $\Delta x \Delta p \geq \frac{\hbar}{2}$.) Further physical motivation for such conjecture (1.3) is loosely based on the fact that there semiclassically is one bound state per phase space area times Planck's constant $\hbar$ [1–3]. See also Gromov's symplectic non-squeezing theorem [4, 5]. The product of uncertainties in various examples is also discussed in, e.g. Ref. [6].

Here we are assuming that the system has a large number of bound states, so that we can apply semiclassical methods. [On top of the bound states, the system could have a continuum of non-normalizable states, which we are not pursuing here. In this article, we are only interested in the bound states below the continuum limit E_0. Note that E_0 could be $+\infty$.]

The conjecture in its basic form (1.3) turns out to be false for at least three reasons (which however may be fixed):

1. Firstly, it is easy to violate any upper bound $C_{\max}$ with a double-well potential with the two wells separated sufficiently far apart. The remedy is to avoid quantum mechanical tunneling, i.e. to impose that the classically accessible region should be connected, cf. Eq. (5.3). With this assumption (along with some minor technical assumptions, Sect. 5), we shall show that an upper bound is $C_{\max} = 1$, cf. Theorem 6.1. Incidentally, this upper bound is saturated for the harmonic oscillator (1.1), cf. Eq. (7.12).
2. Secondly, it is possible to violate any non-zero lower bound $C_{\min}$ with an attractive negative power law potential of the form $\Phi(x) \propto |x|^{\epsilon-2}$, where $\epsilon > 0$ is an arbitrary small number, cf. Appendix B. The reason is that the spectrum of the Hamiltonian is not bounded from below for $\epsilon < 0$. Thus close to the unitarity limit $\epsilon \to 0^+$, it is possible to pack arbitrarily many bound states down the potential throat and saturate the theoretical Heisenberg uncertainty bound $\Delta x \Delta p \geq \frac{\hbar}{2}$. The remedy is to assume that the potential is bounded from below $\Phi(x) \geq V_0 > -\infty$.
3. Thirdly, even for a potential that is bounded from below $\Phi(x) \geq V_0 > -\infty$, any non-zero lower bound $C_{\min}$ may be violated at finite $N \gg 1$, cf. e.g. the two-stage infinite well discussed in Appendix E. The remedy is to consider the infinite $N \to \infty$ limit. With these assumptions, we shall show that an lower bound is $C_{\min} = \frac{\pi}{2\sqrt{3}} \approx 0.9069$, cf. Theorem (6.2). Incidentally, this lower bound is saturated for the infinite square well (1.2).

2. Introduction to WKB

Consider a 1D system with a Hamiltonian of the form

$$H(x,p) = \frac{p^2}{2m} + \Phi(x), \quad x, p \in \mathbb{R}, \tag{2.1}$$

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where $\Phi : \mathbb{R} \to \mathbb{R}$ denotes the potential energy function. For the N-th bound state, where the label $N \gg 1$ is large, we can use semiclassical WKB approximation methods, cf. [1–3]. Semiclassically, the number of states $N = N(E)$ below the energy-level E is given by the area of phase space that is classically accessible, divided by Planck's constant h,

$$N(E) \approx \iint_{H(x,p)\leq E} \frac{\mathrm{d}x\,\mathrm{d}p}{h} = \frac{2}{h}\int_{\Phi(x)\leq E} |p(x)|\,\mathrm{d}x, \quad (2.2)$$

where

$$|p(x)| := \sqrt{2m(E-\Phi(x))} \geq 0. \quad (2.3)$$

Since we are only interested in the semiclassical regime, we ignored in Eq. (2.2) the Maslov index, also known as the metaplectic correction. (The $\approx$ signs are here to remind us of the semiclassical approximation that we made.) The time-independent Schrödinger equation (TISE) is invariant under complex conjugation, so we may assume that the bound state wave functions are real. The WKB wave function $\psi(x)$ for the N-th bound state with energy E reads

$$\psi(x) \approx \frac{C}{\sqrt{|p(x)|}} \cos\left(\frac{S(x)}{\hbar} + \theta\right), \quad (2.4)$$

where

$$S(x) := \int_0^x \mathrm{d}x' |p(x')|, \quad C \in \mathbb{C}, \quad \theta \in \mathbb{R}. \quad (2.5)$$

For further justification of the WKB method, we refer to Ref. [2].

3. Classically accessible length

Let

$$V_0 := \inf_{x\in\mathbb{R}} \Phi(x) \quad (3.1)$$

be the infimum of the potential energy. (V_0 could be $-\infty$.) Let

$$\ell(V) := \lambda(\{x \in \mathbb{R} \mid \Phi(x) \leq V\}) \quad (3.2)$$

be the length of the classically accessible position region at potential energy-level V. Technically, the length $\ell(V)$ is the Lebesgue measure m of the preimage

$$\Phi^{-1}(]-\infty, V]) := \{x \in \mathbb{R} \mid \Phi(x) \leq V\}, \quad (3.3)$$

which in principle does not necessarily have to be a connected interval, although we will later make this assumption, cf. Sect. 5. The accessible length must grow with increasing potential energy

$$\frac{\mathrm{d}\ell(V)}{\mathrm{d}V} \equiv \ell'(V) \geq 0. \quad (3.4)$$

The lower potential energy limit

$$V_0 = \lim_{2x\to 0^+} \ell^{-1}(\{2x\}) \quad (3.5)$$

satisfies

$$\ell(V_0) = 0. \quad (3.6)$$

The continuum limit is

$$E_0 := \lim_{2x\to\infty} \ell^{-1}(\{2x\}). \quad (3.7)$$

We are interested in energies $E \in [V_0, E_0]$. The immaterial factor 2 that appears in Eqs. (3.5) and (3.7) is spurred by an assumption (5.3), which is made later in Sect. 5.

The accumulated accessible length $\mathcal{L}(V)$ at potential energy-level V is defined as:

$$\mathcal{L}(V) := \int_{V_0}^{V} \ell(V')\,\mathrm{d}V'. \quad (3.8)$$

Theorem 3.1. (Abel-like integral transform between $\mathbf{N(E)} \sim \mathbf{I(E)}$ and $\boldsymbol{\ell}\mathbf{(V)}$)

The number $N(E)$ of bound states with energy $\leq E$ can be reconstructed from the accessible length $\ell(V)$ via the formula

$$N(E) \approx \frac{\sqrt{2m}}{h} I(E) \equiv \frac{1}{\pi\hbar}\sqrt{\frac{m}{2}} I(E), \quad (3.9)$$

where $I(E)$ is an integral

$$I(E) := 2\int_{\Phi(x)\leq E} \sqrt{E-\Phi(x)}\,\mathrm{d}x$$
$$= 2\int_{V_0}^{E} \sqrt{E-V}\,\ell'(V)\,\mathrm{d}V \overset{(3.6)}{=} \int_{V_0}^{E} \frac{\ell(V)\,\mathrm{d}V}{\sqrt{E-V}}. \quad (3.10)$$

Conversely, the accumulated accessible length $\mathcal{L}(V)$ at potential energy level V can be reconstructed from $I(E)$ via the formula

$$\mathcal{L}(V) = \frac{1}{\pi}\int_{V_0}^{V} \frac{I(E)\,\mathrm{d}E}{\sqrt{V-E}}$$
$$= \frac{2}{\pi}\int_{V_0}^{V} \mathrm{d}E\, I'(E)\sqrt{V-E}. \quad (3.11)$$

By differentiation of Eq. (3.11), the accessible length $\ell(V)$ at potential energy level V can be reconstructed from $I(E)$ via the formula

$$\ell(V) \equiv \frac{\mathrm{d}\mathcal{L}(V)}{\mathrm{d}V} = \frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}V}\int_{V_0}^{V} \frac{I(E)\,\mathrm{d}E}{\sqrt{V-E}}$$
$$= \frac{1}{\sqrt{\pi}}(D^{\frac{1}{2}}I)(V) = \frac{1}{\pi}\int_{V_0}^{V} \frac{I'(E)\,\mathrm{d}E}{\sqrt{V-E}}. \quad (3.12)$$

Here $D^{\frac{1}{2}}$ denotes a fractional derivative, $(D^{\frac{1}{2}})^2 = D \equiv \frac{\mathrm{d}}{\mathrm{d}V}$.

Proof of Eq. (3.9):

$$hN(E) \overset{(2.2)}{\approx} 2\int_0^{\sqrt{2m(E-V_0)}} \ell\left(E - \frac{p^2}{2m}\right)\mathrm{d}|p| \quad (3.13)$$

$$\overset{V=E-\frac{p^2}{2m}}{=} 2\int_{V_0}^{E} \frac{\ell(V)\,\mathrm{d}V}{v} = \sqrt{2m}\int_{V_0}^{E} \frac{\ell(V)\,\mathrm{d}V}{\sqrt{E-V}}$$
$$\overset{(3.10)}{=} \sqrt{2m}\, I(E), \quad (3.14)$$

because $\mathrm{d}V = -v\,\mathrm{d}|p|$ with speed $v := \frac{|p|}{m} = \sqrt{\frac{2(E-V)}{m}}$.

Proof of Eq. (3.11):

Notice that

$$\int_{V'}^{V} \frac{\mathrm{d}E}{\sqrt{(V-E)(E-V')}}$$
$$\overset{E=V\sin^2\theta+V'\cos^2\theta}{=} 2\int_0^{\frac{\pi}{2}} \mathrm{d}\theta = \pi. \quad (3.15)$$

Then

$$\int_{V_0}^{V} \frac{I(E)\,\mathrm{d}E}{\sqrt{V-E}} \overset{(3.10)}{=} \int_{V_0}^{V} \frac{\mathrm{d}E}{\sqrt{V-E}} \int_{V_0}^{E} \frac{\ell(V')\,\mathrm{d}V'}{\sqrt{E-V'}}$$
$$\overset{\text{Tonelli}}{=} \int_{V_0}^{V} \ell(V')\,\mathrm{d}V' \int_{V'}^{V} \frac{\mathrm{d}E}{\sqrt{(V-E)(E-V')}}$$
$$\overset{(3.15)}{=} \pi \int_{V_0}^{V} \ell(V')\,\mathrm{d}V' \overset{(3.8)}{=} \pi\mathcal{L}(V), \tag{3.16}$$

where we rely on Tonelli's theorem to change the order of integrations.

4. Momentum averages

We will use the notation $\langle F\rangle$ to denote the expectation value of some observable F in the N-th bound state. The momentum average

$$\langle p\rangle = 0 \tag{4.1}$$

is automatically zero. The momentum square average becomes

$$\langle p^2\rangle = \int_{\Phi(x)\le E} |\hbar\psi'(x)|^2\,\mathrm{d}x$$
$$\overset{(2.4)}{\approx} |C|^2 \int_{\Phi(x)\le E} |p(x)| \sin^2\left(\frac{S(x)}{\hbar}+\theta\right)\mathrm{d}x$$
$$\approx \frac{|C|^2}{2} \int_{\Phi(x)\le E} |p(x)|\,\mathrm{d}x \tag{4.2}$$

in the semiclassical limit $|S(x)| \gg \hbar$. Therefore

$$\frac{2\langle p^2\rangle}{|C|^2} \overset{(4.2)}{\approx} \int_{\Phi(x)\le E} |p(x)|\,\mathrm{d}x$$
$$\overset{(2.3)+(3.10)}{=} \sqrt{\frac{m}{2}} I \overset{(3.9)}{\approx} \frac{h}{2}N. \tag{4.3}$$

Similarly, the normalization of the wave function ψ yields

$$\frac{2}{|C|^2} \overset{(2.4)}{\approx} \int_{\Phi(x)\le E} \frac{\mathrm{d}x}{|p(x)|}$$
$$\overset{(2.3)+(4.5)}{=} \frac{J}{\sqrt{2m}} \overset{(3.9)}{\approx} \frac{h}{2m}\frac{\mathrm{d}N}{\mathrm{d}E}, \tag{4.4}$$

where $J(E)$ is an integral

$$J(E) := \int_{\Phi(x)\le E} \frac{\mathrm{d}x}{\sqrt{E-\Phi(x)}}$$
$$= \int_{V_0}^{E} \frac{\ell'(V)\,\mathrm{d}V}{\sqrt{E-V}} = I'(E). \tag{4.5}$$

5. Assumptions

At this stage, to ease calculations, we will from now on make two simplifying assumptions:

1. The potential Φ is an *even* function
$$\Phi(x) = \Phi(-x). \tag{5.1}$$
Then the position average
$$\langle x\rangle = 0 \tag{5.2}$$
is zero.

2. For all potential energy levels V, the classically accessible region is *connected*, i.e. an interval. Then $\mathrm{sgn}(\Phi'(x)) = \mathrm{sgn}(x)$, and the accessible length (3.2) becomes
$$\ell(V) = 2\Phi^{-1}(V) \tag{5.3}$$
i.e. twice the positive inverse branch of Φ. Moreover, the continuum limit (3.7) becomes simply
$$E_0 = \sup_{x\in\mathbb{R}} \Phi(x). \tag{5.4}$$

Then the formulae for the uncertainties reduce to

$$(\Delta x)^2 \overset{(5.2)}{=} \langle x^2\rangle \quad \text{and} \quad (\Delta p)^2 \overset{(4.1)}{=} \langle p^2\rangle. \tag{5.5}$$

The position square average becomes

$$\frac{2\langle x^2\rangle}{|C|^2} \overset{(2.4)}{\approx} \int_{\Phi(x)\le E} \frac{x^2\,\mathrm{d}x}{|p(x)|} \overset{(2.3)+(5.7)}{=} \frac{K}{4\sqrt{2m}}, \tag{5.6}$$

where $K(E)$ is an integral

$$K(E) := \int_{\Phi(x)\le E} \frac{(2x)^2\,\mathrm{d}x}{\sqrt{E-\Phi(x)}} = \int_{V_0}^{E} \frac{\ell(V)^2\ell'(V)\,\mathrm{d}V}{\sqrt{E-V}}$$
$$= \int_{V_0}^{E} \frac{\mathrm{d}V}{3\sqrt{E-V}} \frac{\mathrm{d}\ell(V)^3}{\mathrm{d}V}. \tag{5.7}$$

The second equality in Eq. (5.7) uses assumption 1 and, in particular, assumption 2. Then the product of uncertainties reads

$$U := \frac{\Delta x \Delta p}{\hbar N} \approx \frac{\pi}{\sqrt{2}J}\sqrt{\frac{K}{I}}, \tag{5.8}$$

where we used Eqs. (4.3), (4.4), (5.5), and (5.6). Note that the product (5.8) of uncertainties only depends on the three integrals I, J, and K, which are defined in Eqs. (3.10), (4.5), and (5.7), respectively.

6. Main theorems

We are now ready to state the two main theorems.

Theorem 6.1. (Upper bound)

Given assumptions 1 and 2, then the product (5.8) of uncertainties satisfy the following inequality for large $N \gg 1$:

$$U \lesssim 1 \quad \text{for} \quad N \gg 1. \tag{6.1}$$

Theorem 6.2. (Lower bound)

Given assumptions 1 and 2, and if the potential is bounded from below $\Phi(x) \ge V_0 > -\infty$, then the product (5.8) of uncertainties satisfy the following inequality in the infinite $N \to \infty$ limit:

$$U \gtrsim \frac{\pi}{2\sqrt{3}} \approx 0.9069 \quad \text{for} \quad N \to \infty. \tag{6.2}$$

We stress that the upper bound (6.1) holds for finite $N \gg 1$, while this is not necessarily the case for the lower bound (6.2). See Appendix D for a counterexample.

We believe that the qualitative picture remains the same if we remove assumptions 1, and to some extend, assumption 2.

7. Extremal profile

Note that the independent variable is the derivative $\ell'(V)$ rather than $\ell(V)$ due to the inequality (3.4). The first variations read

$$\delta I \overset{(3.10)}{=} \int_{V_0}^{E} \frac{\delta\ell(V)\,\mathrm{d}V}{\sqrt{E-V}} = 2\int_{V_0}^{E} \sqrt{E-V}\,\delta\ell'(V)\,\mathrm{d}V$$

$$= -2\int_{V_0}^{E}\frac{\mathrm{d}V}{\sqrt{E-V}}\frac{\mathrm{d}}{\mathrm{d}V}\left[(E-V)\delta\ell(V)\right], \tag{7.1}$$

$$\delta J \overset{(4.5)}{=} \int_{V_0}^{E}\frac{\delta\ell'(V)\,\mathrm{d}V}{\sqrt{E-V}} \overset{(7.6)}{=} -\int_{V_0}^{E}\frac{\delta\ell(V)\,\mathrm{d}V}{2(E-V)^{\frac{3}{2}}}, \tag{7.2}$$

$$\delta K \overset{(5.7)}{=} \int_{V_0}^{E}\frac{\mathrm{d}V}{\sqrt{E-V}}\frac{\mathrm{d}}{\mathrm{d}V}\left[\ell(V)^2\delta\ell(V)\right]$$

$$\overset{(7.6)}{=} -\int_{V_0}^{E}\frac{\ell(V)^2\delta\ell(V)\,\mathrm{d}V}{2(E-V)^{\frac{3}{2}}}. \tag{7.3}$$

The second variations read

$$\delta^2 I \overset{(3.10)}{=} 0 \overset{(4.5)}{=} \delta^2 J \tag{7.4}$$

(since I and J are linear in ℓ), and

$$\delta^2 K = 2\int_{V_0}^{E}\frac{\mathrm{d}V}{\sqrt{E-V}}\frac{\mathrm{d}}{\mathrm{d}V}\left[\ell(V)\delta\ell(V)^2\right]$$

$$\overset{(7.6)}{=} -\int_{V_0}^{E}\frac{\ell(V)\delta\ell(V)^2\,\mathrm{d}V}{(E-V)^{\frac{3}{2}}} \leq 0. \tag{7.5}$$

[Note that the rewritings of Eqs. (7.2)–(7.5) in terms of $\frac{\delta\ell(V)}{(E-V)^{\frac{3}{2}}}$ are only integrable/meaningful at the upper limit $V=E$ if we assume the boundary condition

$$\delta\ell(V=E) = 0, \tag{7.6}$$

which we usually will not assume.] Equations (7.1)–(7.3) yield the first variation

$$\frac{\delta U}{U} \overset{(5.8)}{=} \frac{\delta K}{2K} - \frac{\delta I}{2I} - \frac{\delta J}{J}$$

$$= \int_{V_0}^{E}\frac{\mathrm{d}V}{\sqrt{E-V}}\frac{\mathrm{d}}{\mathrm{d}V}\left[g(V)\delta\ell(V)\right]$$

$$= \int_{V_0}^{E}\frac{g(V)\delta\ell'(V)\,\mathrm{d}V}{\sqrt{E-V}} + \int_{V_0}^{E}\frac{g'(V)\,\mathrm{d}V}{\sqrt{E-V}}\int_{V_0}^{V}\mathrm{d}V'\delta\ell'(V')$$

$$= \int_{V_0}^{E}\mathrm{d}V\,\delta\ell'(V)\left[\frac{g(V)}{\sqrt{E-V}} + \int_{V}^{E}\frac{g'(V')\,\mathrm{d}V'}{\sqrt{E-V'}}\right], \tag{7.7}$$

where we have defined

$$g(V) := \frac{\ell(V)^2}{2K} + \frac{E-V}{I} - \frac{1}{J}. \tag{7.8}$$

From Eq. (7.7) with $\ell'(V)$ as independent variable in the variation, we conclude that the Euler–Lagrange equation reads

$$\frac{g(V)}{\sqrt{E-V}} + \int_{V}^{E}\frac{g'(V')\,\mathrm{d}V'}{\sqrt{E-V'}} = 0. \tag{7.9}$$

Differentiation of Eq. (7.9) with respect to V yields

$$\frac{\mathrm{d}}{\mathrm{d}V}\left[\frac{g(V)}{\sqrt{E-V}}\right] = \frac{g'(V)}{\sqrt{E-V}}, \tag{7.10}$$

which in turn leads to that an extremal profile satisfies

$$g(V) = 0. \tag{7.11}$$

Recalling the definition (7.8), the square $\ell_*(V)^2$ of the extremal profile must be affine in V. (Here the subscript "$*$" denotes extremality.) Together with the boundary condition (3.6) this then implies that the extremal profile is

$$\ell_*(V) = A\sqrt{V-V_0}, \quad A>0, \tag{7.12}$$

which corresponds to a harmonic oscillator $\Phi_*(x) - V_0 = \left(\frac{2x}{A}\right)^2 \propto x^2$, i.e. a quadratic potential. The extremal value for the three pertinent integrals are

$$I_* \overset{(3.10)+(7.12)}{=} A\int_{V_0}^{E}\frac{\sqrt{V-V_0}\,\mathrm{d}V}{\sqrt{E-V}}$$

$$\overset{(7.16)}{=} A(E-V_0)B\left(\frac{3}{2},\frac{1}{2}\right) = \frac{\pi}{2}A(E-V_0), \tag{7.13}$$

$$J_* \overset{(4.5)+(7.12)}{=} \frac{A}{2}\int_{V_0}^{E}\frac{\mathrm{d}V}{\sqrt{V-V_0}\sqrt{E-V}}$$

$$\overset{(7.16)}{=} \frac{A}{2}B\left(\frac{1}{2},\frac{1}{2}\right) = \frac{\pi}{2}A, \tag{7.14}$$

$$K_* \overset{(5.7)+(7.12)}{=} \frac{A^3}{2}\int_{V_0}^{E}\frac{\sqrt{V-V_0}\,\mathrm{d}V}{\sqrt{E-V}}$$

$$\overset{(7.16)}{=} \frac{A^3}{2}(E-V_0)B\left(\frac{3}{2},\frac{1}{2}\right) = \frac{\pi}{4}A^3(E-V_0), \tag{7.15}$$

by substitution $v \mapsto V = (E-V_0)v + V_0$. Here

$$B(x,y) = \int_0^1 \mathrm{d}v\,v^{x-1}(1-v)^{y-1} = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)},$$

$$\mathrm{Re}(x), \mathrm{Re}(y) > 0, \tag{7.16}$$

is the Euler beta function. The extremal profile (7.12) saturates the inequality of the upper bound Theorem 6.1

$$U_* \overset{(5.8)+(7.12)}{=} 1. \tag{7.17}$$

8. Proof of the upper bound Theorem 6.1

To prove the upper bound Theorem 6.1, we need to check that the Hessian is negative semidefinite. At the stationary point, we have

$$0 = \frac{\delta U}{U_*} \overset{(5.8)}{=} \frac{\delta K}{2K_*} - \frac{\delta I}{2I_*} - \frac{\delta J}{J_*}, \tag{8.1}$$

or equivalently

$$\frac{\delta K}{K_*} = \frac{\delta I}{I_*} + 2\frac{\delta J}{J_*}. \tag{8.2}$$

Using the Cauchy–Schwarz inequality, we derive

$$(\delta I)^2 \overset{(7.1)}{=} \left[\int_{V_0}^{E}\frac{\delta\ell(V)\,\mathrm{d}V}{\sqrt{E-V}}\right]^2$$

$$\overset{\mathrm{CS-ineq.}}{\leq} \int_{V_0}^{E}\frac{\sqrt{E-V}\,\mathrm{d}V}{\sqrt{V-V_0}}\int_{V_0}^{E}\frac{\sqrt{V-V_0}\,\delta\ell(V)^2\,\mathrm{d}V}{(E-V)^{\frac{3}{2}}}$$

$$\overset{(7.5)+(7.12)}{=} -\frac{\pi}{2}\frac{E-V_0}{A}\delta^2 K, \tag{8.3}$$

or equivalently

$$\left(\frac{\delta I}{I_*}\right)^2 \overset{(7.13)+(7.15)+(8.3)}{\leq} -\frac{\delta^2 K}{2K_*}. \tag{8.4}$$

Therefore the second variation becomes

$$\frac{\delta^2 U}{U_*} \overset{(7.7)}{=} \left(\frac{\delta U}{U_*}\right)^2 + \frac{\delta^2 K}{2K_*} - \frac{1}{2}\left(\frac{\delta K}{K_*}\right)^2 + \frac{1}{2}\left(\frac{\delta I}{I_*}\right)^2$$

$$+ \left(\frac{\delta J}{J_*}\right)^2 \overset{(8.1)}{=} \frac{\delta^2 K}{2K_*} - \left(2\frac{\delta I}{I_*} + \frac{\delta J}{J_*}\right)\frac{\delta J}{J_*}$$

$$\overset{(8.4)}{\leq} -\left(\frac{\delta I}{I_*}+\frac{\delta J}{J_*}\right)^2 \leq 0. \tag{8.5}$$

Moreover, one may show that the only two zero-modes of the Hessian correspond to the two parameters A and V_0 of the harmonic potential (7.12). We conclude that the harmonic potentials (7.12) as the only profiles yield the global maximum for U.

9. Hard wall potentials

A *hard wall potential* is by definition a potential Φ where the classically accessible length ℓ is bounded, i.e. $\exists L<\infty \forall V>V_0 : \ell(V)\leq L$.

Lemma 9.1. (Hard wall potentials)

If the classically accessible length is bounded and the potential is bounded from below $\Phi(x)\geq V_0>-\infty$, then

$$\lim_{E\to\infty} U(E) \overset{(5.8)}{=} \frac{\pi}{2\sqrt{3}} \approx 0.9069. \tag{9.1}$$

Sketched proof of Lemma 9.1:

Equation (9.2) below follows directly from Lebesgue majorant theorem (LMT) using the second integral expression in Eq. (3.10):

$$\lim_{E\to\infty} \frac{I(E)}{\sqrt{E}} \overset{(3.10)}{=} \lim_{E\to\infty} 2\int_{V_0}^{E} \sqrt{1-\frac{V}{E}}\,\ell'(V)\,\mathrm{d}V$$

$$= 2\int_{V_0}^{\infty} \ell'(V)\,\mathrm{d}V = 2\ell(\infty) < \infty. \tag{9.2}$$

[Note that it is easy to construct counterexamples to Eq. (9.2) if $V_0=-\infty$. Such counterexamples typically violate unitarity.] Similarly,

$$\lim_{E\to\infty} \sqrt{E}J(E) \overset{(4.5)}{=} \lim_{E\to\infty} \int_{V_0}^{E} \frac{\ell'(V)\,\mathrm{d}V}{\sqrt{1-\frac{V}{E}}}$$

$$= \int_{V_0}^{\infty} \ell'(V)\,\mathrm{d}V = \ell(\infty), \tag{9.3}$$

$$\lim_{E\to\infty} \sqrt{E}K(E) \overset{(5.7)}{=} \lim_{E\to\infty} \int_{V_0}^{E} \frac{\ell(V)^2\ell'(V)\,\mathrm{d}V}{\sqrt{1-\frac{V}{E}}}$$

$$= \int_{V_0}^{\infty} \ell(V)^2\ell'(V)\,\mathrm{d}V = \frac{\ell(\infty)^3}{3}. \tag{9.4}$$

Equations (9.3) and (9.4) do not follow directly from LMT per se, but possible (likely unphysical) counterexamples are beyond the scope of this article. Equation (9.1) is now a consequence of Eqs. (5.8), (9.2), (9.3), and (9.4).

10. Bounded potentials

Lemma 10.1. (Bounded Potentials)

If the potential is bounded $-\infty<V_0\leq\Phi(x)\leq E_0<\infty$, then

$$U \gtrsim \frac{\pi}{2\sqrt{3}} \approx 0.9069 \quad \text{for} \quad N\gg 1. \tag{10.1}$$

Sketched proof of Lemma 10.1:

Recall that we are still making the assumptions from Sect. 5 for simplicity. Bounded potentials are best analyzed directly in terms of the function $0\leq x\mapsto\Phi(x)$ rather than the inverse function $V_0\leq V\mapsto\ell(V)$ (up to factors of two). The independent variable in the variation is the derivative $\Phi'(x)\geq 0$ for $x\geq 0$. The extremal profiles are finite square wells (C.1), with the position $x=L/2$ of the (positive) kink as the only zero mode, which leads to the estimate (10.1), cf. Appendix C.

Finally, The lower bound Theorem 6.2 follows by use of Lemma 9.1 and Lemma 10.1, and the fact that there is no local minimum in the interior, cf. Sects. 7–8.

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Appendix A: Example: positive power laws

Let the potential be a positive power law

$$\Phi(x) = A\left(\frac{|x|}{L}\right)^{\frac{1}{\alpha}} + V_0, \tag{A.1}$$

with $\alpha, A, L>0$ and $V,E\geq V_0$. Then the accessible length becomes

$$\ell(V) = 2L\left(\frac{V-V_0}{A}\right)^{\alpha}. \tag{A.2}$$

The three integrals can be expressed in terms of the Euler beta function (7.16):

$$I \overset{(3.10)}{=} 2L\frac{(E-V_0)^{\alpha+\frac{1}{2}}}{A^{\alpha}} B\left(\alpha+1,\frac{1}{2}\right), \tag{A.3}$$

$$J \overset{(4.5)}{=} 2\alpha L\frac{(E-V_0)^{\alpha-\frac{1}{2}}}{A^{\alpha}} B\left(\alpha,\frac{1}{2}\right), \tag{A.4}$$

$$K \overset{(5.7)}{=} 8\alpha L^3\frac{(E-V_0)^{3\alpha-\frac{1}{2}}}{A^{3\alpha}} B\left(3\alpha,\frac{1}{2}\right). \tag{A.5}$$

Thus the product of uncertainties becomes

$$U \overset{(5.8)}{\approx} \frac{\pi}{B(\alpha+1,\frac{1}{2})}\sqrt{\frac{B(3\alpha,\frac{1}{2})}{2(\alpha+\frac{1}{2})B(\alpha,\frac{1}{2})}}$$

$$\text{for} \quad N\gg 1. \tag{A.6}$$

The relevant poles in the Euler gamma function (7.16) are

$$B\left(\alpha,\frac{1}{2}\right) \sim \frac{1}{\alpha} \quad \text{for} \quad \alpha\to 0, \tag{A.7}$$

and (via the Stirling formula)

$$B\left(\alpha,\frac{1}{2}\right) \sim \sqrt{\frac{\pi}{\alpha}} \quad \text{for} \quad \alpha\to\infty. \tag{A.8}$$

Remarks:

1. Positive power laws (A.6) respect the upper and lower bounds of the main theorems from Sect. 6.
2. The infinite square well (1.2) corresponds to $\alpha=0$ with $U=\frac{\pi}{2\sqrt{3}}\approx 0.9069$.

3. The harmonic oscillator (1.1) corresponds to $\alpha = \frac{1}{2}$ with $U = 1$.

4. The shallow potential corresponds to $\alpha = \infty$ with $U = \sqrt{\frac{\pi}{2\sqrt{3}}} \approx 0.9523$.

Appendix B: Example: negative power laws

Let the potential be a negative (attractive) power law

$$\Phi(x) = E_0 - A\left(\frac{L}{|x|}\right)^{\frac{1}{\alpha}}, \tag{B.1}$$

with $\alpha > \frac{1}{2}$, $A, L > 0$, $V, E < E_0$, and $V_0 = -\infty$. (One may show that the energy spectrum corresponding to $0 < \alpha < \frac{1}{2}$ is unbounded from below, i.e. the system has no ground state. Hence we only consider $\alpha > \frac{1}{2}$.) The accessible length becomes

$$\ell(V) = 2L\left(\frac{A}{|E_0 - V|}\right)^{\alpha}, \quad V < E_0. \tag{B.2}$$

The three integrals can again be expressed in terms of the Euler beta function (7.16):

$$I \overset{(3.10)}{=} 2L\frac{A^{\alpha}}{|E_0 - E|^{\alpha-\frac{1}{2}}} B\left(\alpha - \frac{1}{2}, \frac{1}{2}\right), \tag{B.3}$$

$$J \overset{(4.5)}{=} 2\alpha L\frac{A^{\alpha}}{|E_0 - E|^{\alpha+\frac{1}{2}}} B\left(\alpha + \frac{1}{2}, \frac{1}{2}\right), \tag{B.4}$$

$$K \overset{(5.7)}{=} 8\alpha L^3\frac{A^{3\alpha}}{|E_0 - E|^{3\alpha+\frac{1}{2}}} B\left(3\alpha + \frac{1}{2}, \frac{1}{2}\right). \tag{B.5}$$

Note that $N \propto I \to \infty$ for $|E_0 - E| \to 0$, so that there are infinitely many bound states for negative power laws (B.1). (On top of that, there is a continuum of non-normalizable states $E > E_0$ with which we are not interested in here.)

Thus the product of uncertainties becomes

$$U \overset{(5.8)}{\approx} \frac{\pi}{B(\alpha - \frac{1}{2}, \frac{1}{2})}\sqrt{\frac{B(3\alpha + \frac{1}{2}, \frac{1}{2})}{2(\alpha - \frac{1}{2})B(\alpha + \frac{1}{2}, \frac{1}{2})}} \quad \text{for} \quad N \gg 1. \tag{B.6}$$

Remarks:

1. Negative power laws (B.6) respect the upper but not the lower bounds of the main theorems from Sect. 6. (The lower bound does not apply since $V_0 = -\infty$.)

2. The shallow potential corresponds to $\alpha = \infty$ with $U = \sqrt{\frac{\pi}{2\sqrt{3}}} \approx 0.9523$, as we found previously.

3. The inverse square potential corresponds to $\alpha = \frac{1}{2}$ with $U = 0$. This is the threshold to quantum mechanically unstable Hamiltonians with spectrum unbounded from below. By going close to $\alpha = \frac{1}{2}$, it is possible to hide as many bound states (as we would like) down the throat, and compress them down to the theoretical limit given by the Heisenberg uncertainty principle (HUP).

Appendix C: Example: finite square well

The finite square well is

$$\Phi(x) = V_0 + (E_0 - V_0)\theta(L - 2|x|) = \begin{cases} V_0 & \text{for} \quad |x| < \frac{L}{2}, \\ E_0 & \text{for} \quad |x| > \frac{L}{2}, \end{cases} \tag{C.1}$$

where $V_0 < E_0$ and $L > 0$. The accessible length becomes

$$\ell(V) \overset{(5.3)}{=} L\theta(V - V_0) + \infty\theta(V - E_0) = \begin{cases} 0 & \text{for} \quad V < V_0, \\ L & \text{for} \quad V_0 < V < E_0, \\ \infty & \text{for} \quad V > E_0, \end{cases} \tag{C.2}$$

where we adopt the convention that $\infty \times 0 = 0$. The three integrals become

$$I(E) \overset{(3.10)}{=} 4\int_0^{\Phi^{-1}(E)} \sqrt{E - \Phi(x)}\,\mathrm{d}x \overset{(C.11)}{=} 2L\sqrt{E - V_0}, \quad V_0 \le E < E_0, \tag{C.3}$$

$$J(E) \overset{(4.5)}{=} 2\int_0^{\Phi^{-1}(E)} \frac{\mathrm{d}x}{\sqrt{E - \Phi(x)}} \overset{(C.1)}{=} \frac{L}{\sqrt{E - V_0}}, \quad V_0 \le E < E_0, \tag{C.4}$$

$$K(E) \overset{(5.7)}{=} 8\int_0^{\Phi^{-1}(E)} \frac{x^2\,\mathrm{d}x}{\sqrt{E - \Phi(x)}} \overset{(C.1)}{=} \frac{L^3}{3\sqrt{E - V_0}}, \quad V_0 \le E < E_0. \tag{C.5}$$

Thus the product of uncertainties becomes

$$U \overset{(5.8)}{\approx} \frac{\pi}{2\sqrt{3}} \approx 0.9069, \quad V_0 \le E < E_0. \tag{C.6}$$

Semiclassically, the product (C.6) of uncertainties for the finite square well agrees (not surprisingly) with the infinite square well (1.2).

Appendix D: Example: a two-stage infinite well

The accessible length is

$$\ell(V) = \sum_{i=0}^{1} L_i\theta(V - V_i) = \begin{cases} 0 & \text{for} \ V < V_0, \\ L_0 & \text{for} \ V_0 < V < V_1, \\ L_0 + L_1 & \text{for} \ V > V_1, \end{cases} \quad L_0, L_1 \ge 0, \quad V_0 \le V_1, \tag{D.1}$$

where θ denotes the Heaviside step function. Equation (D.1) corresponds to a two-stage infinite well potential

$$\Phi(x) = V_0 + (V_1 - V_0)\theta(2|x| - L_0) + \infty\theta(2|x| - L_0 - L_1) = \begin{cases} V_0 & \text{for} \ |x| < \frac{L_0}{2}, \\ V_1 & \text{for} \ \frac{L_0}{2} < |x| < \frac{L_0 + L_1}{2}, \\ \infty & \text{for} \ |x| > \frac{L_0 + L_1}{2}. \end{cases} \tag{D.2}$$

The three integrals become

$$I(E) \overset{(3.10)}{=} 2\sum_{i=0}^{1} L_i\sqrt{E - V_i}\,\theta(E - V_i), \tag{D.3}$$

$$J(E) \stackrel{(4.5)}{=} \sum_{i=0}^{1} L_i \frac{\theta(E-V_i)}{\sqrt{E-V_i}}, \tag{D.4}$$

$$K(E) \stackrel{(5.7)}{=} \frac{L_0^3}{3} \frac{\theta(E-V_0)}{\sqrt{E-V_0}} + \frac{(L_0+L_1)^3 - L_0^3}{3} \frac{\theta(E-V_1)}{\sqrt{E-V_1}}. \tag{D.5}$$

For fixed energy level $E > V_1$ and running $V_0 \to -\infty$, the three pertinent integrals become

$$\lim_{V_0 \to -\infty} \frac{I}{\sqrt{-V_0}} \stackrel{(D.3)}{=} 2L_0, \tag{D.6}$$

$$\lim_{V_0 \to -\infty} J \stackrel{(D.4)}{=} \frac{L_1}{\sqrt{E-V_1}}, \quad E > V_1, \tag{D.7}$$

$$\lim_{V_0 \to -\infty} K \stackrel{D.5}{=} \frac{(L_0+L_1)^3 - L_0^3}{3\sqrt{E-V_1}}, \quad E > V_1, \tag{D.8}$$

The product (5.8) of uncertainties $U \to 0$ vanishes in that limit

$$\lim_{V_0 \to -\infty} U \stackrel{(5.8)}{=} 0, \quad E > V_1, \quad L_1 > 0. \tag{D.9}$$

Equation (D.9) shows that there is in general no nonzero lower bound for the product (5.8) of uncertainties U for finite energy E even if the potential is bounded from below $\Phi(x) \geq V_0 > -\infty$.

Appendix E: Example: logarithmic potentials

Let the accessible length be of the form

$$\ell(V) = P(V-V_0)e^{\alpha(V-V_0)} = P\left(\frac{\mathrm{d}}{\mathrm{d}\alpha}\right) \mathrm{e}^{\alpha(V-V_0)},$$

$$\ell'(V) = P\left(\frac{\mathrm{d}}{\mathrm{d}\alpha}\right) \alpha\, \mathrm{e}^{\alpha(V-V_0)}, \tag{E.1}$$

where $\alpha > 0$ is a positive constant and $P(z) = \sum_{k=0}^{m} a_k z^k$ is a polynomial with root $z = 0$ (so that $\ell(V_0) = 0$). Let the energy level $E > V_0$ be arbitrary but fixed. We are interested in the shallow potential limit $\alpha \to \infty$. Concretely, let us assume that

$$\alpha \gg \frac{1}{E-V_0}. \tag{E.2}$$

The three integrals then become Gaussian

$$I \stackrel{(3.10)+(E.1)}{=} P\left(\frac{\mathrm{d}}{\mathrm{d}\alpha}\right) \int_{V_0}^{E} \frac{\mathrm{e}^{\alpha(V-V_0)}\,\mathrm{d}V}{\sqrt{E-V}}$$

$$\stackrel{y=\sqrt{E-V}}{=} 2P\left(\frac{\mathrm{d}}{\mathrm{d}\alpha}\right) \mathrm{e}^{\alpha(E-V_0)} \int_0^{\sqrt{E-V_0}} \mathrm{e}^{-\alpha y^2}\,\mathrm{d}y$$

$$\stackrel{(E.2)}{\approx} P\left(\frac{\mathrm{d}}{\mathrm{d}\alpha}\right) \mathrm{e}^{\alpha(E-V_0)} \sqrt{\frac{\pi}{\alpha}} \stackrel{(E.2)}{\approx} \ell(E)\sqrt{\frac{\pi}{\alpha}}. \tag{E.3}$$

Similarly,

$$J \stackrel{(4.5)+(E.1)+(E.2)}{\approx} \ell(E)\sqrt{\pi\alpha}, \tag{E.4}$$

and

$$K \stackrel{(5.7)+(E.1)+(E.2)}{\approx} \ell(E)^3 \sqrt{\frac{\pi\alpha}{3}}. \tag{E.5}$$

Note that $N \propto I \to \infty$ for $E \to \infty$, so that such logarithmic potentials (E.1) have infinitely many bound states. The product (5.8) of uncertainties becomes

$$U \stackrel{(5.8)+(E.1)+(E.2)}{\approx} \sqrt{\frac{\pi}{2\sqrt{3}}} \approx 0.9523 \text{ for } N \gg 1. \tag{E.6}$$

Note that the (E.6) of uncertainties has universal features in the sense that it does not depend on the parameters E, V_0, α (as long as Eq. (E.2) is satisfied), nor the polynomial P. The value (E.6) sits right in the middle of the double inequality.

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