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ABSTRACT

We complete our study on the uncertainties in position and momentum associated with the semiclassical Hagedorn wave packets by first filling in a technical gap in the dynamics of bound states for isochronous potentials. We then consider scattered states and show that, if the packet is reflected from the potential or transmitted through a symmetric potential, then a minimal uncertainty "initial" state cannot in general lead to a "final" state with minimal uncertainty, and we give an explicit relationship for the difference in terms of a characteristic time associated with classical trajectories. We also characterize the behavior of the uncertainty product in the case where the underlying classical dynamics lead to capture by the potential.

I. INTRODUCTION

This work completes a previous study[1] by the authors on the dynamics of the position and momentum uncertainties for semiclassical wave packets. We extend our previous results on bound states to scattered and captured states, and we close a gap in a result on the attaining of minimal uncertainty for bound states at energies where the period is locally independent of the energy.

The wave packets under consideration are the Hagedorn[2] states $\{\varphi_n\}$.

Definition 1. For $n \in \mathbb{Z}^+ \cup \{0\}$, $a, \eta \in \mathbb{R}$, $\hbar > 0$, and $A, B \in \mathbb{C}$ satisfying

$$A\overline{B} + \overline{A}B = 2, \tag{1}$$

we let

$$\begin{aligned}\varphi_n(A,B,\hbar,a,\eta,x) = {} & 2^{-n/2}(n!)^{-1/2}(\pi\hbar)^{-1/4}A^{-(n+1)/2}\overline{A}^{n/2} \\ & \times H_n\left(\hbar^{-1/2}|A|^{-1}(x-a)\right) \\ & \times \exp\left\{-\frac{1}{2\hbar}BA^{-1}(x-a)^2 + \frac{i}{\hbar}\eta(x-a)\right\},\end{aligned}$$

where H_n is the n^{th} order Hermite polynomial.

With $\langle\cdot,\cdot\rangle$ and $\|\cdot\|$ denoting the inner product and norm for $L^2(\mathbb{R}, dx)$, given $\psi(x) \in L^2(\mathbb{R}, dx)$ normalized so that

$$\langle\psi,\psi\rangle = \|\psi\|^2 = \int_{-\infty}^{\infty} |\psi(x)|^2\, dx = 1,$$

the expectations $\langle x\rangle$ and $\langle p\rangle$ of position and momentum are given by

$$\langle x\rangle = \langle\psi, x\psi\rangle$$

and

$$\langle p\rangle = \left\langle\psi, (-i\hbar\frac{\partial}{\partial x})\psi\right\rangle.$$

The uncertainties in these quantities are

$$\Delta x = \sqrt{\langle\psi, (x - \langle x\rangle)^2\psi\rangle}$$

and

$$\Delta p = \sqrt{\left\langle\psi, (-i\hbar\frac{\partial}{\partial x} - \langle p\rangle)^2\psi\right\rangle}.$$

The uncertainty principle

$$\Delta x\Delta p \geq \frac{\hbar}{2} \tag{2}$$

follows, and if equality is achieved, we will say that the state ψ is of minimal uncertainty.

The states $\varphi_n(A, B, \hbar, a, \eta, x)$ as defined above are normalized in $L^2(\mathbb{R}, dx)$ and have expected position and momentum

$$\langle x\rangle = a \text{ and } \langle p\rangle = \eta$$

and uncertainties

$$\Delta x = \sqrt{\hbar\left(n + \frac{1}{2}\right)}|A| \text{ and } \Delta p = \sqrt{\hbar\left(n + \frac{1}{2}\right)}|B|.$$

Consistent with (2), it follows easily from condition (1) that $|A||B| \geq 1$.

II. BOUND STATES

The Hagedorn states provide semiclassical solutions for the Schrödinger equation. For example, suppose that $V \in C^2(\mathbb{R}, \mathbb{R})$ is bounded from below and such that $|V(x)| \leq Ce^{Mx^2}$ for some constants C and M so that $H = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2} + V(x)$ generates a unitary propagator $U(t) = e^{-itH/\hbar}$ on $L^2(\mathbb{R}, dx)$. Let

$$\begin{aligned}\varphi(\hbar, x, t) &= e^{iS(t)/\hbar}\varphi_0(A(t), B(t), \hbar, a(t), \eta(t), x)\\ &= (\pi\hbar)^{-1/4}A(t)^{-1/2}\exp\left\{-\frac{1}{2\hbar}B(t)A(t)^{-1}(x - a(t))^2\right.\\ &\quad\left.+\frac{i}{\hbar}\eta(t)(x - a(t)) + \frac{i}{\hbar}S(t)\right\},\end{aligned}$$

where $\{a(t), \eta(t), A(t), B(t), S(t)\}$ is the solution of

$$\dot{a}(t) = \eta(t), \tag{3}$$

$$\dot{\eta}(t) = -V'(a(t)), \tag{4}$$

$$\dot{A}(t) = iB(t), \tag{5}$$

$$i\dot{B}(t) = -V''(a(t))A(t), \tag{6}$$

$$\dot{S}(t) = \frac{1}{2}\eta(t)^2 - V(a(t)) \tag{7}$$

for some initial condition $\{a(0), \eta(0), A(0), B(0), S(0)\} \in \mathbb{R}\times\mathbb{R}\times\mathbb{C}\times\mathbb{C}\times\{0\}$ with $A(0)\overline{B(0)} + \overline{A(0)}B(0) = 2$. Let the branch of the square root of $A(t)$ be determined by continuity in t starting on the principle branch at $t = 0$. Then,[2]

$$\left\| e^{-itH/\hbar}\varphi(\hbar,\cdot,0) - \varphi(\hbar,\cdot,t)\right\| = O(\hbar^{1/2})$$

for t in any compact interval $[0, T]$. Note that (1) is conserved, that is,

$$A(t)\overline{B(t)} + \overline{A(t)}B(t) = 2$$

for $t \geq 0$ and that this particular asymptotic solution $\varphi(\hbar, x, t)$ has expected position and momentum

$$\langle x\rangle = a(t) \text{ and } \langle p\rangle = \eta(t)$$

and uncertainties

$$\Delta x = \sqrt{\frac{\hbar}{2}}|A(t)| \text{ and } \Delta p = \sqrt{\frac{\hbar}{2}}|B(t)|.$$

We recall our earlier results[1] on the evolution of $A(t)$ and $B(t)$.

Proposition 2. Suppose $V \in C^2(\mathbb{R},\mathbb{R})$. Let $\{a(t), \eta(t), A(t), B(t)\}$ be the solution of (3)–(6) for some initial condition $\{a_0, \eta_0, A_0, B_0\} \in \mathbb{R}\times\mathbb{R}\times\mathbb{C}\times\mathbb{C}$ with $A_0\overline{B_0} + \overline{A_0}B_0 = 2$ and such that a_0 is between two adjacent roots $x_- < x_+$ of $V(x) = E$ with $V'(x_-) < 0$ and $V'(x_+) > 0$. Let $\tau(E)$ denote the period of $a(t)$ and $\eta(t)$. Then, if $\tau'(E) = 0$, $A(t)$ and $B(t)$ are periodic with period τ, while if $\tau'(E) \neq 0$, $A(t)$ and $B(t)$ have the form

$$A(t) = A_1(t) + tA_2(t),$$
$$B(t) = B_1(t) + tB_2(t)$$

with A_1, A_2, B_1, and B_2 periodic with period τ.

Proposition 3. Under the hypothesis of Proposition 2, given any $T > 0$, there is a time $t > T$ such that $|A(t)B(t)| = 1$.

Proposition 4. Under the hypothesis of Proposition 2, if $\tau'(E) \neq 0$, then there exists $T > 0$ such that, for any $t_0 > T$, the uncertainty product is minimal ($|A(t)B(t)| = 1$) for at least four times t in the interval $[t_0, t_0 + \tau]$.

Proposition 2 is a result of Floquet theory applied to the system

$$\frac{d}{dt}\begin{bmatrix} A(t) \\ iB(t)\end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -V''(a(t)) & 0\end{bmatrix}\begin{bmatrix} A(t) \\ iB(t)\end{bmatrix},$$

which has the fundamental matrix solution

$$\Phi(t) = \begin{bmatrix} \dfrac{\partial a}{\partial a_0}(t) & \dfrac{\partial a}{\partial \eta_0}(t) \\ \dfrac{\partial \eta}{\partial a_0}(t) & \dfrac{\partial \eta}{\partial \eta_0}(t)\end{bmatrix}$$

and monodromy matrix

$$\Phi(\tau) = \begin{bmatrix} 1 - \eta_0\tau'(E)V'(a_0) & -\eta_0^2\tau'(E) \\ V'(a_0)^2\tau'(E) & 1 + \eta_0\tau'(E)V'(a_0)\end{bmatrix}.$$

Proposition 3 follows from either the periodicity of $A(t)$ and $B(t)$ (if $\tau'(E) = 0$) or the iteration of the monodromy matrix. Our immediate goal is to extend Proposition 4 to the case where $\tau'(E) = 0$.

A. Isochronous potentials

The Proof of Proposition 4 requires the hypothesis that the energy $E = \frac{1}{2}\eta_0^2 + V(a_0)$ is such that $\tau'(E) \neq 0$. Since the conclusion of the proposition is true for the harmonic oscillator ($V(x) = \frac{1}{2}\omega^2 x^2$) which famously has period independent of energy, it is certainly reasonable to question whether this hypothesis is necessary. We will show that indeed it is, that is, there are potentials V and energies E such that $\tau'(E) = 0$ and the uncertainty product is minimal only twice in any interval $[t_0, t_0 + \tau]$.

First, let us verify that Proposition 4 is true for the potential $V(x) = \frac{1}{2}\omega^2 x^2$ which has $\tau'(E) = 0$ for all $E > 0$. We set $\omega = 1$ for convenience. The system (5) and (6) has solution

$$A(t) = A_0 \cos t + iB_0 \sin t,$$
$$B(t) = B_0 \cos t + iA_0 \sin t$$

with period $\tau = 2\pi$. If we set $\Gamma = B_0/A_0$, then, from (1), we have $\mathrm{Re}(\Gamma) = 1/|A_0|^2 > 0$ and

$$A_0 = \frac{1}{\sqrt{\mathrm{Re}(\Gamma)}} e^{i\alpha}, \tag{8}$$

$$B_0 = \frac{\sqrt{\mathrm{Re}(\Gamma)^2 + \mathrm{Im}(\Gamma)^2}}{\sqrt{\mathrm{Re}(\Gamma)}} e^{i(\alpha + \arctan(\mathrm{Im}(\Gamma)/\mathrm{Re}(\Gamma)))} \tag{9}$$

for some $\alpha \in [0, 2\pi)$. From the Proof[1] of Proposition 3, we know that $|A(t)B(t)| = 1$ if and only if $\frac{d}{dt}|A(t)| = 0$. Some algebra now shows that, for this example, $\frac{d}{dt}|A(t)| = 0$ if and only if

$$\left(\mathrm{Re}(\Gamma)^2 + \mathrm{Im}(\Gamma)^2 - 1\right) \sin 2t = 2\,\mathrm{Im}(\Gamma) \cos 2t. \tag{10}$$

Now, if $\mathrm{Im}(\Gamma) = 0$ and $\mathrm{Re}(\Gamma) = 1$, then (10) is true for all t. If $\mathrm{Im}(\Gamma) = 0$ and $\mathrm{Re}(\Gamma) \neq 1$, then (10) is true when $\sin 2t = 0$, that is, four times per period. If $\mathrm{Im}(\Gamma) \neq 0$, then (10) is true at times t such that either $\cos 2t = 0$ (if $\mathrm{Re}(\Gamma)^2 + \mathrm{Im}(\Gamma)^2 = 1$) or

$$\tan 2t = \frac{2\,\mathrm{Im}(\Gamma)}{\mathrm{Re}(\Gamma)^2 + \mathrm{Im}(\Gamma)^2 - 1}$$

(if $\mathrm{Re}(\Gamma)^2 + \mathrm{Im}(\Gamma)^2 \neq 1$), so $\frac{d}{dt}|A(t)| = 0$ occurs four times per period.

We now give heuristic, numeric, and finally analytic evidence for the existence of potentials for which $\tau'(E) = 0$ for one or more values of E, yet $\frac{d}{dt}|A(t)| = 0$ occurs fewer than four times per period. We begin with a "half-oscillator," namely, $V(x) = \frac{1}{2}x^2$ on $x > 0$ with a reflecting boundary condition at $x = 0$. The explicit solution of (3) and (4) with $a_0 > 0$ and a reflection at the origin is

$$a(t) = |a_0 \cos t + \eta_0 \sin t|,$$
$$\eta(t) = (\eta_0 \cos t - a_0 \sin t)\,\mathrm{sgn}(a_0 \cos t + \eta_0 \sin t),$$

which has period π. Setting

$$A(t) = \frac{\partial a}{\partial a_0} A_0 + i\frac{\partial a}{\partial \eta_0} B_0 = (A_0 \cos t + iB_0 \sin t)\,\mathrm{sgn}(a_0 \cos t + \eta_0 \sin t)$$

and following the argument above, using (8) and (9) leads to exactly Eq. (10). However, now the underlying period is half that of before, so we conclude $\frac{d}{dt}|A(t)| = 0$ twice per period. Of course, this example violates more of our hypotheses than we like.

For $\alpha \in (0, 1)$, the potential[3]

$$V(x) = \frac{2 + (1+\alpha)(x^2 + 2x) - 2(x+1)\sqrt{1 + \alpha x(x+2)}}{2(1-\alpha)^2} \tag{11}$$

on $(-\infty, \infty)$ is isochronous with $\tau(E) = 2\pi$ for all $E > 0$. From numerical experiments with various initial conditions, it seems that the uncertainty product is usually minimal four times per period, but for values of α near one and certain initial conditions $\{a_0, \eta_0, A_0, B_0\}$ (e.g., $\alpha = 0.99$, $\{a_0, \eta_0, A_0, B_0\} = \{0, 1, 1, \sqrt{2}e^{-i\pi/4}\}$), the numerical solution of (3)–(6) reveals that the uncertainty product is minimal only twice per period.

As $\alpha \to 1$, the potential (11) converges[3] on $(0, \infty)$ to

$$V(x) = \frac{1}{2}x^2 + \frac{1}{2x^2}.$$

We can explicitly solve Eqs. (3)–(6) for this potential. Using a standard trick[4] for Ermakov equations, we have

$$a(t) = \frac{1}{\sqrt{2}a_0}\sqrt{a_0^4 + a_0^2\eta_0^2 + 1 + \left(a_0^4 - a_0^2\eta_0^2 - 1\right)\cos 2t + 2a_0^3\eta_0 \sin 2t}$$

for $a_0 > 0$ and we can construct $\eta(t)$, $A(t)$, and $B(t)$ by differentiating this with respect to time or initial conditions. From this, we can construct exact solutions for which the uncertainty product is minimal only twice in any period. The initial conditions $\{a_0, \eta_0, A_0, B_0\} = \{2, 0, 1, 1\}$ provide once such example, where $\tau = \pi$,

$$|A(t)| = \frac{1}{8}\sqrt{\frac{995 + 1020\cos 2t + 33\cos 4t}{17 + 15\cos 2t}},$$

and $\frac{d}{dt}|A(t)|$ has zeroes at $t = n\pi/2$ for integer n. Introducing a smooth cutoff at some appropriate $\varepsilon > 0$ does not affect this solution $\{a, \eta, A, B\}$ for energies $E < V(\varepsilon)$, so we can use this example to construct a potential satisfying the assumptions of Proposition 2 with $\{a, \eta, A, B\}$ such that minimality of the uncertainty product occurs only twice in any period.

Therefore, the assumption $\tau'(E) \neq 0$ is indeed necessary to ensure minimality of the uncertainty product at least four times per period and we can extend Proposition 4 to include the $\tau'(E) = 0$ case. In this case, $|A(t)| = |A(t+\tau)|$, so we know by the mean value theorem that $\frac{d}{dt}|A(t)| = 0$ at least once per period. Letting t^* be any such time, a further application of the mean value theorem gives $\frac{d}{dt}|A(t)| = 0$ somewhere between t^* and $t^* + \tau$. Hence, we can replace Proposition 4 by the following:

Proposition 5. Under the hypothesis of Proposition 2, if $\tau'(E) \neq 0$, then there exists $T > 0$ such that, for any $t_0 > T$, the uncertainty product is minimal ($|A(t)B(t)| = 1$) for at least four times t in the interval $[t_0, t_0 + \tau]$. If $\tau'(E) = 0$, then the uncertainty product is minimal at least twice during any period.

III. SEMICLASSICAL SCATTERING

We now consider a semiclassical scattering process that maps a state asymptotic to a Gaussian wave packet ψ_- at $t = -\infty$ into a similar state ψ_+ at $t = \infty$. Our focus is on the associated uncertainties $\Delta x_\pm$ and $\Delta p_\pm$ in position and momentum, respectively, of these states. We show that, if the packet is reflected from the potential or transmitted through a symmetric potential, then a minimal uncertainty "initial" state ($\Delta x_- \Delta p_- = \hbar/2$) cannot in general lead to a "final" state with minimal uncertainty, that is, $\Delta x_+ \Delta p_+ > \hbar/2$, and we give an explicit relationship for the difference in terms of a characteristic time. We also analyze the behavior of the uncertainty product in the case where the underlying classical dynamics lead to capture by the potential.

We consider the classical Hamiltonian

$$H(a, \eta) = \frac{1}{2}\eta^2 + V(a)$$

on $\mathbb{R}^2$ and its quantum counterpart

$$H(\hbar) = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2} + V(x) = H_0(\hbar) + V(x)$$

on $L^2(\mathbb{R})$ for "short range" potentials $V \in C^3(\mathbb{R})$ satisfying

$$\left|\frac{d^j V}{dx^j}(x)\right| \leq d_j(1 + |x|)^{-1-j-\nu} \tag{12}$$

for some constants d_j, $j \in \{0, 1, 2, 3\}$, and some $\nu > 0$.

We first collect some results on one-dimensional classical and quantum scattering. From the work of Hagedorn[2] and the references therein,[5–9] for all $\hbar > 0$, $H(\hbar)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R})$, the wave operators

$$\Omega^\pm(\hbar) = s - \lim_{t \to \mp\infty} e^{itH(\hbar)/\hbar} e^{-itH_0(\hbar)/\hbar}$$

exist and are asymptotically complete, and the quantum S-matrix given by $\mathbf{S}(\hbar) = \Omega^-(\hbar) * \Omega^+(\hbar)$ is unitary. Given $(a_-, \eta_-) \in \mathbb{R}^2$ with $\eta_- \neq 0$, there exists a unique solution $(a(t), \eta(t))$ of the classical system

$$\dot{a}(t) = \eta(t),$$
$$\dot{\eta}(t) = -V'(a(t))$$

such that

$$\lim_{t\to-\infty}|a(t)-a_--t\eta_-|=0 \tag{13}$$

and

$$\lim_{t\to-\infty}|\eta(t)-\eta_-|=0. \tag{14}$$

On the other hand, there is a closed set $\mathcal{E}\subset\{(a_-,\eta_-)\in\mathbb{R}^2:\eta_-\neq 0\}$ of measure zero such that for $(a_-,\eta_-)\notin\mathcal{E}$ there exist a_+ and $\eta_+\neq 0$ such that

$$\lim_{t\to\infty}|a(t)-a_+-t\eta_+|=0 \tag{15}$$

and

$$\lim_{t\to\infty}|\eta(t)-\eta_+|=0. \tag{16}$$

The classical S-matrix $\mathbf{S}_{cl}:\mathbb{R}^2/\mathcal{E}\to\mathbb{R}^2$ is defined by the mapping

$$\mathbf{S}_{cl}(a_-,\eta_-)=(a_+,\eta_+).$$

From Theorem 1.2 of Hagedorn,[2] given $(a_-,\eta_-)\in\mathbb{R}^2/\mathcal{E}$ and $A_-,B_-\in\mathbb{C}$ satisfying

$$A_-\overline{B_-}+\overline{A_-}B_-=2,$$

there exist $a_+,\eta_+,S_+\in\mathbb{R}$ with $\eta_+\neq 0$, $A_+,B_+\in\mathbb{C}$, and a unique solution of the system (3)–(7) such that Eqs. (13)–(16) hold along with the following:

$$\lim_{t\to\pm\infty}|A(t)-A_\pm-itB_\pm|=0,$$
$$\lim_{t\to\pm\infty}|B(t)-B_\pm|=0,$$

$$\lim_{t\to-\infty}\left|S(t)-\frac{1}{2}t\eta_-^2\right|=0,$$

$$\lim_{t\to\infty}\left|S(t)-S_+-\frac{1}{2}t{\eta_+}^2\right|=0,$$

$$A(t)=\frac{\partial a(t)}{\partial a_-}A_-+i\frac{\partial a(t)}{\partial\eta_-}B_-,$$
$$B(t)=\frac{\partial\eta(t)}{\partial\eta_-}B_--i\frac{\partial\eta(t)}{\partial a_-}A_-,$$

$$A(t)\overline{B(t)}+\overline{A(t)}B(t)=2, \tag{17}$$

$$A_+=\frac{\partial a_+}{\partial a_-}A_-+i\frac{\partial a_+}{\partial\eta_-}B_-, \tag{18}$$

$$B_+=\frac{\partial\eta_+}{\partial\eta_-}B_--i\frac{\partial\eta_+}{\partial a_-}A_-, \tag{19}$$

and

$$A_+\overline{B_+}+\overline{A_+}B_+=2. \tag{20}$$

The main result of Theorem 1.2 of Ref. 2 is that, for any $\lambda\in\left(0,\frac{1}{2}\right)$, if we consider the coherent state φ_0, namely,

$$\varphi_0(A,B,\hbar,a,\eta,x)=(\pi\hbar)^{-1/4}A^{-1/2}\exp\left\{-\frac{1}{2\hbar}BA^{-1}(x-a)^2+\frac{i}{\hbar}\eta(x-a)\right\},$$

then, with the appropriate choice for the branch of the square root of A_+,

$$\left\|\mathbf{S}\varphi_0(A_-,B_-,\hbar,a_-,\eta_-,\cdot)-e^{iS_+/\hbar}\varphi_0(A_+,B_+,\hbar,a_+,\eta_+,\cdot)\right\|=O(\hbar^\lambda).$$

Remark 6. *Hagedorn*[2] *proved his Theorem 1.2 for spatial dimension $n \geq 3$. Rothstein*[10] *provided the necessary estimates for the extension to one and two dimensions.*

A. The asymptotic uncertainties

We now turn our attention to understanding the effect of scattering on the uncertainties, that is, we begin our focus on the relationship $(A_-, B_-) \to (A_+, B_+)$. We consider three separate physical cases, namely, reflection from, transmission through, and capture by the potential. For the first two cases, we will consider a_- and $\eta_- \neq 0$ such that $(a_-, \eta_-) \in \mathbb{R}^2/\mathcal{E}$. The classical S-matrix $\mathbf{S}_{cl} : \mathbb{R}/\mathcal{E} \to \mathbb{R}$ is the mapping

$$\mathbf{S}_{cl}(a_-, \eta_-) = (a_+, \eta_+),$$

and its Jacobian matrix

$$\Phi_+ = \Phi_+(a_-, \eta_-) = \begin{bmatrix} \dfrac{\partial a_+}{\partial a_-} & \dfrac{\partial a_+}{\partial \eta_-} \\ \dfrac{\partial \eta_+}{\partial a_-} & \dfrac{\partial \eta_+}{\partial \eta_-} \end{bmatrix} \tag{21}$$

serves to scatter the uncertainties in the sense that

$$\begin{bmatrix} A_+ \\ iB_+ \end{bmatrix} = \Phi_+(a_-, \eta_-) \begin{bmatrix} A_- \\ iB_- \end{bmatrix}.$$

By conservation of energy and $\lim_{t\to\infty} V(a(t)) = 0$,

$$\eta_+ = \pm\eta_-,$$

so

$$\frac{\partial \eta_+}{\partial \eta_-} = \pm 1,$$
$$\frac{\partial \eta_+}{\partial a_-} = 0.$$

Then, Eqs. (18)–(20) with $A_- = B_- = 1$ imply

$$\frac{\partial a_+}{\partial a_-} = \pm 1,$$

and therefore,

$$\Phi_+ = \Phi_+(a_-, \eta_-) = \begin{bmatrix} \pm 1 & \dfrac{\partial a_+}{\partial \eta_-} \\ 0 & \pm 1 \end{bmatrix}$$

and

$$A_+ = \pm A_- + i\frac{\partial a_+}{\partial \eta_-} B_-,$$
$$B_+ = \pm B_-.$$

We first consider reflection off the potential ($\eta_+ = -\eta_-$) followed by transmission through the potential ($\eta_+ = \eta_-$). We then will allow (a_-, η_-) in the exceptional set and study the trapping of particles by the potential.

1. Reflection

We consider a particle reflecting off the potential. For an incoming particle,

$$a(t) \sim a_- + t\eta_-,$$
$$\eta(t) \sim \eta_-$$

as $t \to -\infty$ with $(a_-, \eta_-) \in \mathbb{R}^2/\mathcal{E}$ and energy $E = \frac{1}{2}\eta_-^2 < \max_{x\in\mathbb{R}} V(x)$, we define the arrival time $\tau = \tau(a_-, \eta_-)$ by $\eta(\tau) = 0$, that is,

$$\eta(a_-,\eta_-,\tau(a_-,\eta_-)) = 0.$$

The hypotheses on V are sufficient to guarantee continuity of $\frac{\partial\eta}{\partial a_-}$, $\frac{\partial\eta}{\partial\eta_-}$, and $\frac{\partial\eta}{\partial t}$; hence the implicit function theorem guarantees that τ is well-defined and has continuous partial derivatives with respect to a_- and η_-. We exploit the fact that the phase space trajectory $(a(t),\eta(t))$ is symmetric about the arrival time, that is,

$$a(\tau+t) = a(\tau-t),$$
$$\eta(\tau+t) = -\eta(\tau-t)$$

to obtain, as $t\to\infty$,

$$a_+ + (\tau+t)\eta_+ \sim a(\tau+t) = a(\tau-t) \sim a_- + (\tau-t)\eta_-,$$

so

$$a_+ = a_- + 2\tau\eta_-$$

and the classical scattering matrix is

$$\mathbf{S}_{cl}(a_-,\eta_-) = (a_+,\eta_+) = (a_- + 2\tau\eta_-, -\eta_-). \tag{22}$$

The matrix Φ_+ defined by (21) is then

$$\Phi_+ = \begin{bmatrix} -1 & 2\dfrac{\partial}{\partial\eta_-}(\tau\eta_-) \\ 0 & -1 \end{bmatrix}. \tag{23}$$

Note that

$$\frac{\partial a_+}{\partial a_-} = -1 \Rightarrow \frac{\partial\tau}{\partial a_-} = -\frac{1}{\eta_-},$$

so

$$\tau(a_-,\eta_-) = F(\eta_-) - \frac{a_-}{\eta_-}$$

for some function F and therefore

$$\frac{\partial}{\partial a_-}\left(\frac{\partial}{\partial\eta_-}(\tau\eta_-)\right) = 0,$$

so Φ_+ is a function of η_- alone.

If we now consider scattering a minimal uncertainty state, that is, we consider a state of the form $\varphi_0(A_-, B_-, \hbar, a_-, \eta_-, x)$ with

$$|A_-||B_-| = 1,$$

then from the above and the fact that, from (1),

$$|A_-||B_-| = |\overline{A_-}B_-| = \sqrt{1+\mathrm{Im}(\overline{A_-}B_-)^2} \Rightarrow \mathrm{Im}(\overline{A_-}B_-) = 0,$$

with some algebra, we obtain

$$|A_+||B_+| = \sqrt{1+4\left(\frac{\partial}{\partial\eta_-}(\tau\eta_-)\right)^2|B_-|^2},$$

and hence, we see that the semiclassically scattered state

$$\varphi_0(A_+,B_+,\hbar,a_+,\eta_+,x)$$

is also of minimal uncertainty if and only if $\eta_- = \eta_-^*$ satisfies

$$\left.\left(\frac{\partial}{\partial\eta_-}(\tau\eta_-)\right)\right|_{\eta_-^*} = 0. \tag{24}$$

We collect these results as a Proposition.

Proposition 7. With the assumptions and definitions in Secs. III and III A, for $(a_-, \eta_-) \in \mathbb{R}^2/\mathcal{E}$ *with* $|\eta_-| < \max_{x\in\mathbb{R}} V(x)$, *define* $\tau = \tau(a_-, \eta_-)$ *by*

$$\eta(a_-, \eta_-, \tau(a_-, \eta_-)) = 0.$$

Then,

$$\Phi_+ = \Phi_+(\eta_-) = \begin{bmatrix} -1 & 2\dfrac{\partial}{\partial\eta_-}(\tau\eta_-) \\ 0 & -1 \end{bmatrix}$$

and

$$\begin{aligned} A_+ &= -A_- + 2i\left(\frac{\partial}{\partial\eta_-}(\tau\eta_-)\right)B_-, \\ B_+ &= -B_-. \end{aligned}$$

Furthermore, if $|A_-||B_-| = 1$, *then* $|A_+||B_+| = 1$ *if and only if* $\Phi_+ = -I$, *that is, the value of* η_- *is such that* $\frac{\partial}{\partial\eta_-}(\tau\eta_-) = 0$.

a. An example: The Morse potential. We explicitly work out the details above for the Morse potential

$$V(x) = D(1 - e^{-\alpha(x-x_0)})^2 - D,$$

where $D > 0$, $\alpha > 0$, and x_0 are constants. For convenience, we set $x_0 = 0$.

This potential does not satisfy our decay assumption 12, but this is easily overcome since we can restrict ourselves to classical and semiclassical scattering for positive energies less than some $E_{\max}$ and introduce a sufficiently smooth and rapidly decaying cutoff to $V(x)$ for $x < a_{\min}$, where $V(a_{\min}) = E_{\max}$. The classical and semiclassical scattering for particles at positive energy $E < E_{\max}$ incoming from the right will not be affected.

From the known explicit classical dynamics for this potential,[11] we can deduce that, given $a_- \in \mathbb{R}$ and $\eta_- < 0$, the solution of (3) and (4) that satisfies

$$\begin{aligned} a(t) &\sim a_- + \eta_- t, \\ \eta(t) &\sim \eta_- \end{aligned}$$

as $t \to -\infty$ is

$$a(t) = \frac{1}{\alpha}\log\left(2\delta\cosh(\alpha(a_- + t\eta_-) - \log(\delta)) - \frac{2D}{\eta_-^2}\right), \tag{25}$$

$$\eta(t) = \frac{2\delta\eta_- \sinh(\alpha(a_- + t\eta_-) - \log(\delta))}{2\delta\cosh(\alpha(a_- + t\eta_-) - \log(\delta)) - \dfrac{2D}{\eta_-^2}}, \tag{26}$$

where, for the sake of notation, we have set

$$\delta = \frac{\sqrt{D}}{\eta_-^2}\sqrt{D + \frac{1}{2}\eta_-^2}.$$

It follows then by taking limits of (25) and (26) as $t \to \infty$,

$$\begin{aligned} a(t) &\sim a_+ + \eta_+ t, \\ \eta(t) &\sim \eta_+, \end{aligned}$$

where $\eta_+ = -\eta_-$ and

$$a_+ = -a_- + \frac{1}{\alpha}\log\left(\frac{D}{\eta_-^4}\left(D + \frac{1}{2}\eta_-^2\right)\right).$$

The classical S-matrix $\mathbf{S}_{cl} : \{(a_-, \eta_-) : \eta_- < 0\} \to \mathbb{R}^2$ is then

$$\mathbf{S}_{cl}(a_-, \eta_-) = (a_+, \eta_+) = \left(-a_- + \frac{1}{\alpha}\log\left(\frac{D}{\eta_-^4}\left(D + \frac{1}{2}\eta_-^2\right)\right), -\eta_-\right).$$

By explicit calculation,

$$\begin{aligned} A_+ &= \frac{\partial a_+}{\partial a_-}A_- + i\frac{\partial a_+}{\partial \eta_-}B_- = -A_- - i\frac{2(4D + \eta_-^2)}{\alpha\eta_-(2D + \eta_-^2)}B_-, \\ B_+ &= \frac{\partial \eta_+}{\partial \eta_-}B_- - i\frac{\partial \eta_+}{\partial a_-}A_- = -B_-, \end{aligned}$$

and the matrix Φ_+ defined in (21) is

$$\Phi_+ = \begin{bmatrix} \frac{\partial a_+}{\partial a_-} & \frac{\partial a_+}{\partial \eta_-} \\ \frac{\partial \eta_+}{\partial a_-} & \frac{\partial \eta_+}{\partial \eta_-} \end{bmatrix} = -\begin{bmatrix} 1 & \frac{2(4D + \eta_-^2)}{\alpha\eta_-(2D + \eta_-^2)} \\ 0 & 1 \end{bmatrix}.$$

To see that these results agree with (22) and (23), first note that solving $\eta(t) = 0$ gives

$$\begin{aligned} \tau(a_-, \eta_-) &= \frac{1}{\alpha\eta_-}\log(\delta) - \frac{a_-}{\eta_-} \\ &= \frac{1}{2\alpha\eta_-}\log\left(\frac{D}{\eta_-^4}\left(D + \frac{1}{2}\eta_-^2\right)\right) - \frac{a_-}{\eta_-}, \end{aligned}$$

so

$$a_- + 2\tau\eta_- = -a_- + \frac{1}{\alpha}\log\left(\frac{D}{\eta_-{}^4}\left(D + \frac{1}{2}\eta_-^2\right)\right)$$

and

$$\begin{aligned} -2\frac{\partial}{\partial \eta_-}(\tau(a_-, \eta_-)\eta_-) &= -2\frac{\partial}{\partial \eta_-}\left(\frac{1}{2\alpha}\log\left(\frac{D}{\eta_-^4}\left(D + \frac{1}{2}\eta_-^2\right)\right) - a_-\right) \\ &= \frac{2(4D + \eta_-^2)}{\alpha\eta_-(2D + \eta_-^2)}. \end{aligned}$$

2. Transmission and symmetric potentials

In the case of transmission through the potential, we have $\eta_+ = \eta_-$ and

$$\Phi_+ = \begin{bmatrix} 1 & \frac{\partial a_+}{\partial \eta_-} \\ 0 & 1 \end{bmatrix}.$$

For an incoming particle

$$\begin{aligned} a(t) &\sim a_- + t\eta_-, \\ \eta(t) &\sim \eta_- \end{aligned}$$

as $t \to -\infty$ with $(a_-, \eta_-) \in \mathbb{R}^2/\mathcal{E}$ and energy $E = \frac{1}{2}\eta_-^2 > \max_{x\in\mathbb{R}} V(x)$, we define the arrival time $\tau = \tau(a_-, \eta_-)$ in this case by $a(\tau) = 0$, that is,

$$a(a_-, \eta_-, \tau(a_-, \eta_-)) = 0.$$

The hypotheses on V are sufficient to guarantee the continuity of $\frac{\partial a}{\partial a_-}$, $\frac{\partial a}{\partial \eta_-}$, and $\frac{\partial a}{\partial t}$; hence, the implicit function theorem guarantees that τ is well-defined and has continuous partial derivatives with respect to a_- and η_-.

There is not much more we can say here in general. If, however, we consider an even potential $(V(-x) = V(x))$ then we can again exploit a symmetry for

$$a(a_-, \eta_-, \tau + t) = -a(a_-, \eta_-, \tau - t)$$

and

$$\eta(a_-, \eta_-, \tau + t) = \eta(a_-, \eta_-, \tau - t)$$

implying

$$a_+ = -a_- - 2\tau\eta_-,$$

so the classical scattering matrix is

$$\mathbf{S}_{cl}(a_-, \eta_-) = (a_+, \eta_+) = (-a_- - 2\tau\eta_-, \eta_-)$$

and

$$\Phi_+ = \begin{bmatrix} 1 & -2\dfrac{\partial}{\partial \eta_-}(\tau\eta_-) \\ 0 & 1 \end{bmatrix}.$$

Again, we see that Φ_+ is independent of a_-, and if we consider scattering a minimal uncertainty state $\varphi_0(A_-, B_-, \hbar, a_-, \eta_-, x)$ with

$$|A_-||B_-| = 1,$$

we obtain

$$|A_+||B_+| = \sqrt{1 + 4\left(\frac{\partial}{\partial \eta_-}(\tau\eta_-)\right)^2 |B_-|^2},$$

and therefore, the semiclassically scattered state $\varphi_0(A_+, B_+, \hbar, a_+, \eta_+, x)$ is also of minimal uncertainty if and only if $\eta_- = \eta_-^*$ satisfies (24) with τ defined as in this section. In the case of an even potential, we can combine the results of this section with those of the previous to obtain the following:

Proposition 8. Suppose $V = V(|x|)$ satisfies (12). With the assumptions and definitions in Secs. III and III A, for $(a_-, \eta_-) \in \mathbb{R}^2/\mathcal{E}$, define $\tau = \tau(a_-, \eta_-)$ as the time of closest approach to the origin, that is,

$$\frac{d}{dt}|a(a_-, \eta_-, t)|^2\bigg|_{t=\tau(a_-,\eta_-)} = 2a(a_-, \eta_-, \tau(a_-, \eta_-))\eta(a_-, \eta_-, \tau(a_-, \eta_-)) = 0.$$

Then,

$$\Phi_+ = \Phi_+(\eta_-) = \pm\begin{bmatrix} 1 & -2\dfrac{\partial}{\partial \eta_-}(\tau\eta_-) \\ 0 & 1 \end{bmatrix},$$

where the upper sign is chosen in the case of transmission and the lower in the case of reflection. Furthermore, if $|A_-||B_-| = 1$, then $|A_+||B_+| = 1$ if and only if $\Phi_+ = \pm I$, that is, if and only if η_- is such that $\frac{\partial}{\partial \eta_-}(\tau\eta_-) = 0$.

Since τ is given in terms of the asymptotic positions and momenta by

$$\tau = -\frac{1}{2}\left(\frac{a_-}{\eta_-} + \frac{a_+}{\eta_+}\right),$$

we see that τ is related to the notion of classical global time delay[12,13] T,

$$T = \frac{a_-}{\eta_-} - \frac{a_+}{\eta_+}$$
$$= 2\left(\tau + \frac{a_-}{\eta_-}\right);$$

hence,

$$2\frac{\partial}{\partial\eta_-}(\tau\eta_-) = \frac{\partial}{\partial\eta_-}(T\eta_-).$$

The case where $2\frac{\partial}{\partial\eta_-}(\tau\eta_-) = \mp\frac{\partial a_+}{\partial\eta_-} = \frac{\partial}{\partial\eta_-}(T\eta_-) = 0$ for some value(s) of η_- is uncommon. We remark, however, that this condition holds throughout for transmission in the trivial case $V(x) \equiv 0$ and, with some obvious modification in the definition of τ, for reflection off an otherwise constant vertical potential step.

3. Capture by the potential

Finally, for completeness, we will consider the case where the classical particle is captured, for example, at the top of a potential hill (see, for example, Remark 5 in the work of Hagedorn[2] or Appendix 2 in the work of Simon[9]). We first document the long-time asymptotics of $A(t)$ and $B(t)$ if we take a_- and $\eta_- \neq 0$ in the exceptional set and such that the particle comes to rest at the top of a hill, i.e., such that $(a_+, 0)$ is an (unstable) equilibrium solution of the classical motion. In particular, $V'(a_+) = 0$ and $V''(a_+) < 0$. Linearizing (3) and (4) about $(a_+, 0)$ and setting

$$\lambda = \sqrt{-V''(a_+)}$$

gives

$$a(t) \sim a_+ + ce^{-\lambda t},$$
$$\eta(t) \sim -\lambda ce^{-\lambda t}$$

for some constant c as $t \to \infty$. Setting $V''(a(t)) = -\lambda$ in (5) and (6) gives

$$A(t) \sim c_1\cosh(\lambda t) + \frac{i}{\lambda}c_2\sinh(\lambda t),$$
$$B(t) \sim c_2\cosh(\lambda t) - i\lambda c_1\sinh(\lambda t)$$

for some constants c_1 and c_2 which, by (17), satisfy

$$c_1\overline{c_2} + \overline{c_1}c_2 = 2.$$

Both $|A(t)|$ and $|B(t)|$ then must grow exponentially and the uncertainty product follows suit

$$|A(t)B(t)| \sim \frac{e^{2\lambda t}}{4\lambda}|\lambda c_1 + ic_2|^2$$

as $t \to \infty$.

We now consider generalizing to the case where more derivatives vanish at the top of the hill and to the case where the particle is captured on a "ledge." With the particle incident from the right, we therefore wish to consider the higher order Taylor expansion for V about a_+ with the first nonzero term being

$$\frac{1}{n!}V^{(n+1)}(a_+)(a(t) - a_+)^n$$

with $n \geq 2$ and $V^{(n+1)}(a_+) < 0$. With

$$\lambda = \sqrt{-\frac{1}{n!}V^{(n+1)}(a_+)}$$

and $y(t) = a(t) - a_+$, this leads us to study the nonlinear ordinary differential equation

$$\ddot{y} = \lambda^2 y^n \tag{27}$$

with the asymptotic conditions

$$\lim_{t\to\infty} y(t) = 0, \tag{28}$$

$$\lim_{t\to\infty} \dot{y}(t) = 0. \tag{29}$$

Rewriting (27) as

$$\dot{y}\frac{d\dot{y}}{dy} = \lambda^2 y^n,$$

we obtain

$$\frac{\dot{y}^2}{2} = \lambda^2 \frac{y^{n+1}}{n+1} + \text{const.} \tag{30}$$

From (28) and (29), the constant in (30) must be zero and we can separate the resulting equation for $y(t)$ and obtain the solution

$$y(t) = \left(\frac{2(n+1)}{\lambda^2(n-1)^2(t+c)^2}\right)^{\frac{1}{n-1}},$$

where c is an arbitrary constant, and we have used the facts that $y(t) > 0$ and $\dot{y}(t) < 0$ to determine a branch.

If, for the sake of notation, we let

$$\Lambda_n = \left(\frac{2(n+1)!}{|V^{(n+1)}(a_+)|(n-1)^2}\right)^{\frac{1}{n-1}},$$

then the (a, η) dynamics near the capture point look like

$$a(t) \sim a_+ + \frac{\Lambda_n}{t^{2/(n-1)}},$$

$$\eta(t) \sim -\frac{2\Lambda_n}{(n-1)t^{(n+1)/(n-1)}}$$

as $t \to \infty$. The approximate ODE for $A(t)$ is then

$$\ddot{A}(t) - \alpha_n t^{-2} A(t) = 0,$$

where

$$\alpha_n = \frac{2n(n+1)}{(n-1)^2};$$

hence,

$$A(t) = O(t^{(1+\sqrt{1+4\alpha_n})/2})$$

as $t \to \infty$, and therefore, the uncertainty product scales as

$$|A(t)B(t)| \sim O(t^{(\sqrt{1+4\alpha_n})})$$

as $t \to \infty$.

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