Particle in a box uncertainty

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I. PRELIMINARIES

We are interested in uncertainty region, the set

$$U = \left\{ \left(\Delta_\rho^2 \, \mathrm{Q},\ \Delta_\rho^2 \, \mathrm{P}\right) \,\middle|\, \rho \in \mathcal{S}\left(\mathcal{D}\right) \right\} \tag{1}$$

of points defined by the "uncertainty functional"

$$\Delta_\rho^2 \, \mathrm{A} = \left\langle \mathrm{A}^2 \right\rangle_\rho - \left\langle \mathrm{A} \right\rangle_\rho^2 , \tag{2}$$

where $\mathcal{D}$ is the set of norm one elements $\varphi \in L^2([-\pi,\pi])$ which are continuously differentiable, and such that $\varphi'' \in L^2([-\pi,\pi])$ and $\varphi(-\pi) = \varphi(\pi) = 0$[1]. $\mathcal{S}\left(\mathcal{D}\right)$ is the usual space of trace 1, positive semi-definite operators formed by taking convex combinations of projections onto elements of $\mathcal{D}$.

The operators P and Q are defined in the usual way on this space

$$\left(\mathrm{P}\,\varphi\right)(x) = -i\,\varphi'(x) \tag{3}$$
$$\left(\mathrm{Q}\,\varphi\right)(x) = x\,\varphi(x). \tag{4}$$

Note that for any observable A the variance functional is concave in the state. Take ρ, $\sigma \in \mathcal{S}\left(D\right)$ with finite first and second moments of A and choose $\lambda \in (0,1)$ then

$$0 \le \lambda(1-\lambda)\left(\left\langle \mathrm{A} \right\rangle_\rho - \left\langle \mathrm{A} \right\rangle_\sigma\right)^2 \tag{5}$$
$$\lambda^2 \left\langle \mathrm{A} \right\rangle_\rho^2 + (1-\lambda)^2 \left\langle \mathrm{A} \right\rangle_\sigma^2 + 2\lambda(1-\lambda)\left\langle \mathrm{A} \right\rangle_\rho \left\langle \mathrm{A} \right\rangle_\sigma \le \lambda \left\langle \mathrm{A} \right\rangle_\rho^2 + (1-\lambda)\left\langle \mathrm{A} \right\rangle_\sigma^2 \tag{6}$$
$$\left(\lambda \left\langle \mathrm{A} \right\rangle_\rho + (1-\lambda)\left\langle \mathrm{A} \right\rangle_\sigma\right)^2 = \tag{7}$$
$$\left\langle \mathrm{A}^2 \right\rangle_{\lambda\rho+(1-\lambda)\sigma} - \left(\lambda \left\langle \mathrm{A} \right\rangle_\rho + (1-\lambda)\left\langle \mathrm{A} \right\rangle_\sigma\right)^2 \ge \lambda\left(\left\langle \mathrm{A}^2 \right\rangle_\rho - \left\langle \mathrm{A} \right\rangle_\rho^2\right) + (1-\lambda)\left(\left\langle \mathrm{A} \right\rangle_\sigma^2 - \left\langle \mathrm{A} \right\rangle_\sigma^2\right) \tag{8}$$
$$\Delta^2_{\lambda\rho+(1\text{-}\lambda)\sigma} \, \mathrm{A} \ge \lambda\, \Delta_\rho^2 \, \mathrm{A} + (1-\lambda)\, \Delta_\sigma^2 \, \mathrm{A}\,. \tag{9}$$

II. MOMENTUM SHIFT INVARIANCE

It is obvious from the boundary conditions that we do not have the invariance of the state-space under position shifts which allows for significant simplifications when trying to solve the problem on, for example, the entire real line or for the "particle on a ring" system. However we still have invariance under momentum shifts, which can be seen by expressing the effect of the "shift operators" in the position representation

$$(e^{ip\,\mathrm{Q}}\varphi)(x) = e^{ipx}\varphi(x) \tag{10}$$
$$(e^{ip\,\mathrm{Q}}\varphi)(-\pi) = e^{-i\pi p}\varphi(-\pi) = 0 = e^{i\pi p}\varphi(\pi) = (e^{ip\,\mathrm{Q}}\varphi)(\pi). \tag{11}$$

Critically this shift does not change any of the moments of the position observable, or the variance of the momentum observable, so the uncertainty region U is exactly the same as the region

$$R = \left\{ \left(\Delta_\rho^2 \, \mathrm{Q},\ \left\langle \mathrm{P}^2 \right\rangle_\rho\right) \,\middle|\, \rho \in \mathcal{S}\left(\mathcal{D}\right),\ \left\langle \mathrm{P} \right\rangle_\rho = 0 \right\}, \tag{12}$$

obtained by setting the momentum expectation to zero.

III. GLOBAL FACTS ABOUT THE UNCERTAINTY REGION

It is clear that the region is contained in the quadrant with $0 \leq \Delta^2 \mathrm{Q}$, $0 \leq \Delta^2 \mathrm{P}$, further, since the interval is bounded above and below by π and $-\pi$, we must have that $\Delta^2_\rho Q \leq \left\langle Q^2 \right\rangle_\rho \leq \pi^2$.

Take any smooth, L^2 normalised, function $f : \mathbb{R} \to \mathbb{R}$, supported only on $[0, 1]$, and consider

$$g_{a,s}(x) = \frac{1}{\sqrt{2s}} f\left(\frac{x-a}{s}\right) + \frac{1}{\sqrt{2s}} f\left(\frac{-x-a}{s}\right), \tag{13}$$

where a is non-negative, s is positive and they are taken such that $a+s < \pi$. The resulting $g_{a,s}$ is a smooth function supported on $[-a-s, -a] \cup [a, a+s]$, with $\langle \mathrm{Q} \rangle_{g_{a,s}} = 0$, and so has finite momentum variance as well as

$$a^2 < \Delta^2_{\mathrm{g_{a,s}}} \mathrm{Q} < (a+s)^2. \tag{14}$$

By varying a and s in the allowed region we see that in any interval $I = (\alpha, \alpha + \varepsilon) \subset (0, \pi^2)$ there exists some state ρ with $\Delta^2_\rho \mathrm{Q} \in X$. Further, given any two position uncertainties $\Delta^2_\phi \mathrm{Q}$ and $\Delta^2_\psi \mathrm{Q}$, achieved by pure states ϕ and ψ we can define the state

$$\xi_\theta = \frac{1}{\sqrt{1 + 2\cos\theta \sin\theta \,\mathrm{re}\left(\langle \phi | \psi \rangle\right)}} \left(\cos\theta \,\phi + \sin\theta \,\psi\right), \tag{15}$$

and the continuous, real valued function $\theta \mapsto \Delta^2_{\xi_\theta} \mathrm{Q}$. The intermediate value theorem then asserts that for every variance $v \in (\Delta^2_\phi \mathrm{Q}, \Delta^2_\psi \mathrm{Q})$ there exists $\theta^* \in (0, \pi)$ such that $\Delta^2_{\xi_{\theta^*}} \mathrm{Q} = v$.

Given a state we can increase its momentum variance as much as we like, whilst leaving the moments of position unchanged, by applying the following map,

$$M_a : \phi \mapsto \left(x \mapsto \phi(x) e^{aix^2}\right) \tag{16}$$

$$\langle \mathrm{Q}^n \rangle_{M_a \phi} = \langle \mathrm{Q}^n \rangle_\phi \tag{17}$$

$$\Delta^2_{\mathrm{M_a}\phi} \mathrm{P} = \Delta^2_\phi \mathrm{P} + a^2 \Delta^2_\phi \mathrm{Q} - 2a \langle \mathrm{P} \rangle_\phi \langle \mathrm{Q} \rangle_\phi . \tag{18}$$

This means that given some $x \in (0, \pi^2)$ there is exactly one point on the boundary of the uncertainty region with $\Delta^2 \mathrm{Q} = x$. The boundary may therefore be expressed as the graph of a function

$$b : (0, \pi^2) \to (0, \infty) \tag{19}$$

$$b : x \mapsto \inf \left\{ \Delta^2_\rho \mathrm{P} \,\middle|\, \rho \in \mathcal{S}(\mathcal{D}),\, \Delta^2_\rho \mathrm{Q} = x \right\}. \tag{20}$$

The expectation $\left\langle \mathrm{P}^2 \right\rangle_\rho$ has a global minimum at $\frac{1}{4}$, which we can find quite easily as the least eigenvalue of P^2

$$\psi_k(x) = \frac{1}{\sqrt{\pi}} \sin \frac{k+1}{2}(x - \pi), \quad k \in \{0, 1, ...\} \tag{21}$$

$$\mathrm{P}^2 \psi_k = \frac{(k+1)^2}{4} \psi_k \tag{22}$$

$$\inf_\rho \left\langle \mathrm{P}^2 \right\rangle_\rho = \left\langle \mathrm{P}^2 \right\rangle_{\psi_0} = \frac{1}{4} \tag{23}$$

$$\Delta^2_{\psi_0} \mathrm{Q} = \left\langle \mathrm{Q}^2 \right\rangle_{\psi_0} = \frac{\pi^2}{3} - 2 \approx 1.3. \tag{24}$$

The boundary curve must be strictly decreasing for $\Delta^2 \mathrm{Q} < \Delta^2_{\psi_0} \mathrm{Q}$, and strictly increasing for $\Delta^2 \mathrm{Q} > \Delta^2_{\psi_0} \mathrm{Q}$, which may be shown by taking each state on the boundary, setting its momentum expectation to zero, and mixing the resultant state ρ with the minimiser $\sigma = |\psi_0\rangle\langle\psi_0|$. It is easy to see that for each variance $v \in (\Delta^2_{\psi_0} \mathrm{Q}, \Delta^2_\rho \mathrm{Q})$ there exists a $\lambda^* \in (0, 1)$ such that

$$\tau(\lambda) = (1-\lambda)\rho + \lambda\sigma \tag{25}$$

$$\Delta^2_{\tau(\lambda^*)} \mathrm{Q} = v. \tag{26}$$

The existence of the required λ^* can be asserted by noting that $\lambda \mapsto \Delta^2_{\tau(\lambda)}\,\mathrm{Q}$ is continuous, and applying the intermediate value theorem. Since ψ_0 is the unique minimiser of $\langle \mathrm{P}^2 \rangle$ it follows that

$$\begin{aligned} \Delta^2_{\tau(\lambda^*)}\,\mathrm{P} &= \left\langle \mathrm{P}^2 \right\rangle_{\tau(\lambda^*)} && (27)\\ &= (1-\lambda^*)\left\langle \mathrm{P}^2 \right\rangle_{\sigma} + \lambda^* \left\langle \mathrm{P}^2 \right\rangle_{\rho} && (28)\\ &< \left\langle \mathrm{P}^2 \right\rangle_{\rho}, && (29)\end{aligned}$$

which gives the result.

A. Upper and lower bounds

There is an obvious linear isometry $F : \mathcal{D} \to L^2(\mathbb{R})$ which takes each pure state in $\mathcal{D}$ and simply extends it to be zero outside $[-\pi, \pi]$

$$F : \phi \mapsto \left(x \mapsto \begin{cases} \phi(x), & -\pi \le x \le \pi \\ 0, & \text{otherwise} \end{cases} \right). \tag{30}$$

This map will take the position and momentum observables we have defined and map them to the usual $L^2(\mathbb{R})$ position and momentum. in doing so it will not change the variances, and so the canonical hyperbola $\Delta^2\,\mathrm{P}\,\Delta^2\,\mathrm{Q} = \frac{1}{4}$ gives a lower bound for our boundary function

$$b(x) \ge \frac{1}{4x}. \tag{31}$$

If it were the case that the minimal momentum uncertainty for each position uncertainty could be achieved by a state with position expectation zero, then the uncertainty region would be given by

$$X = \left\{ \left(\left\langle \mathrm{Q}^2 \right\rangle_{\rho}, \left\langle \mathrm{P}^2 \right\rangle_{\rho} \right) \,\middle|\, \rho \in \mathcal{S}(\mathcal{D}) \right\}. \tag{32}$$

It is easy to see that this region is convex, and so the boundary may be defined by its Legendre transform, we ask for a set of inequalities of the form

$$\left\langle \mathrm{P}^2 \right\rangle_{\rho} + \alpha \left\langle \mathrm{Q}^2 \right\rangle_{\rho} \ge c(\alpha) \tag{33}$$

for each $\alpha \in \mathbb{R}$. Intuitively we are finding the tangent to the boundary curve at each point and using that the region is convex so each tangent line bounds the region below. Applying the well known functional calculus we see that this amounts to solving the eigenvalue problem

$$\begin{aligned} \mathrm{H}_\alpha\,\varphi_\alpha &= \left(\mathrm{P}^2 + \alpha\,\mathrm{Q}^2\right)\varphi_\alpha = c(\alpha)\varphi_\alpha && (34)\\ \varphi_\alpha(-\pi) &= \varphi_\alpha(\pi) = 0, && (35)\end{aligned}$$

for the least eigenvalue of H_α. The ground states are easy to express in terms of the confluent hyper-geometric function, or in terms of parabolic cylinder functions, however these representations are not very useful for computing the eigenvalue $c(\alpha)$. Instead we use that the eigenstates ψ_k of P^2 form a core for the operators H_α, so that we can compute arbitrarily good approximations to $c(\alpha)$ by expressing the operator as a matrix $h_{n,m} = \langle \psi_n | \mathrm{H}_\alpha\,\psi_m \rangle$, truncating the matrix at some finite dimension, and numerically computing the least eigenvalue for a range of α values.

Once we have a set of points $\{(\alpha_i, c(\alpha_i)) \mid i \in (1, \ldots n)\}$, sufficiently close together we can approximate the derivative $c'(\alpha)$ to get approximations to

$$\begin{aligned} \Delta^2_{\varphi_\alpha}\,\mathrm{Q} &= c'(\alpha) && (36)\\ \Delta^2_{\varphi_\alpha}\,\mathrm{P} &= c(\alpha) - \alpha c'(\alpha). && (37)\end{aligned}$$

Note that although it might be that the boundary is only realised by states with $\langle \mathrm{Q} \rangle \neq 0$ the set of states with $\langle \mathrm{Q} \rangle = 0$ is a subset of $\mathcal{D}$, and so the uncertainties of the states we find in this way are in the uncertainty region, and hence are an upper bound for b.

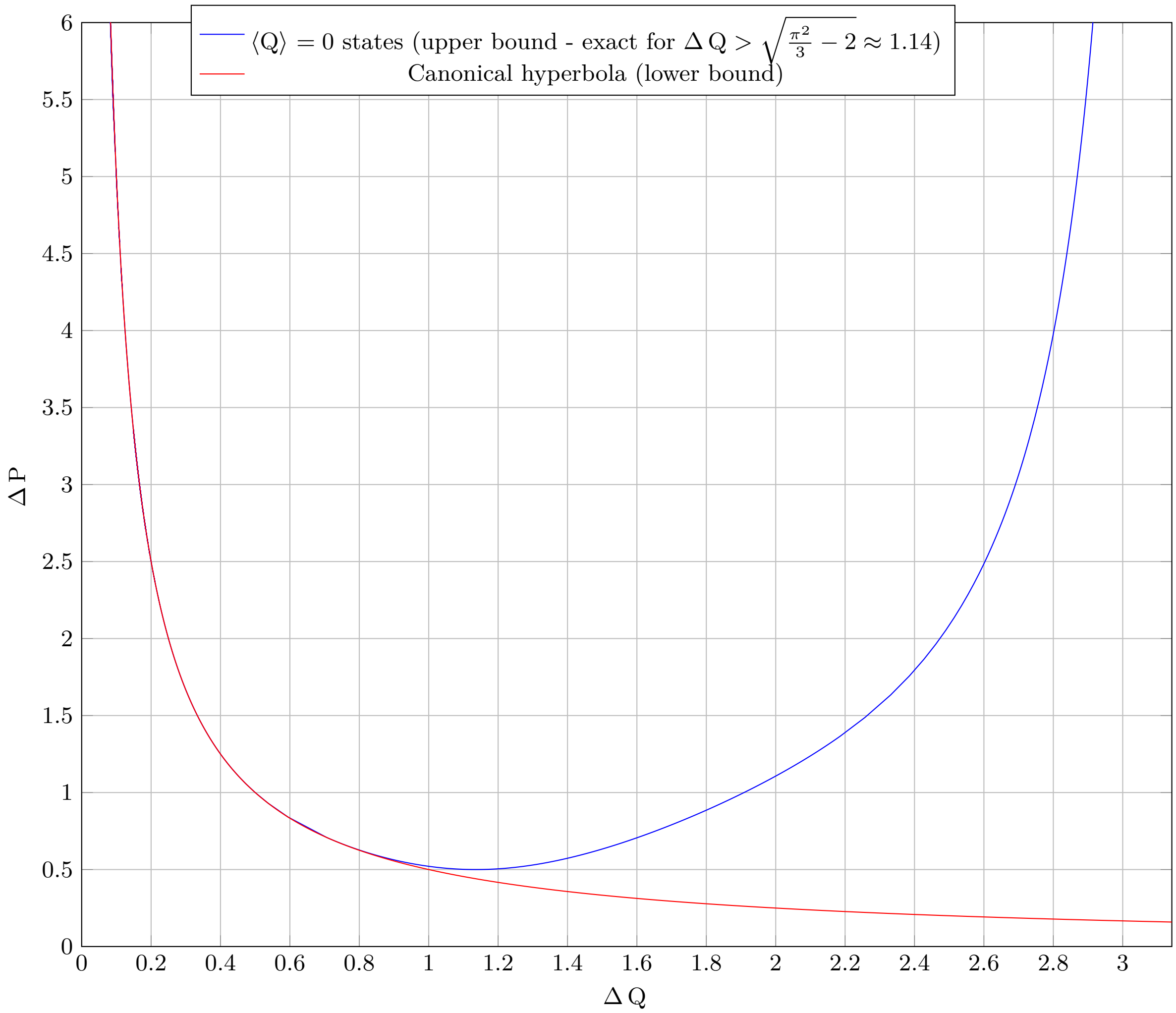

FIG. 1. Plot showing the lower (31) and upper (36), (37) bounds for the uncertainty region boundary, in red and blue respectively. The upper bound is exact for $\Delta\,\mathrm{Q} > \sqrt{\frac{\pi^2}{3}-2} \approx 1.14$, and is conjectured to be exact everywhere.

IV. THE EXACT BOUNDARY CURVE

Given the ground state φ of H_α for some $\alpha \in \mathbb{R}$ assume, there is some state ρ such that

$$\left\langle \mathrm{Q}^2 \right\rangle_\rho - \langle \mathrm{Q} \rangle_\rho^2 = \Delta_\rho^2\,\mathrm{Q} = \Delta_\varphi^2\,\mathrm{Q} = \left\langle \mathrm{Q}^2 \right\rangle_\varphi \tag{38}$$

$$\left\langle \mathrm{P}^2 \right\rangle_\rho < \left\langle \mathrm{P}^2 \right\rangle_\varphi , \tag{39}$$

then

$$\left\langle \mathrm{P}^2 + \alpha\,\mathrm{Q}^2 \right\rangle_\varphi \leq \operatorname{tr}\left(\rho\left(\mathrm{P}^2 + \alpha\,\mathrm{Q}^2\right)\right) \tag{40}$$

$$= \left\langle \mathrm{P}^2 \right\rangle_\rho + \alpha \left\langle \mathrm{Q}^2 \right\rangle_\rho \tag{41}$$

$$= \left\langle \mathrm{P}^2 \right\rangle_\rho + \alpha \left(\left\langle \mathrm{Q}^2 \right\rangle_\varphi + \langle \mathrm{Q} \rangle_\rho^2 \right) \tag{42}$$

$$< \left\langle \mathrm{P}^2 \right\rangle_\varphi + \alpha \left\langle \mathrm{Q}^2 \right\rangle_\varphi + \alpha \langle \mathrm{Q} \rangle_\rho^2 \tag{43}$$

which is an obvious contradiction for $\alpha < 0$, which is the region in which the curve is increasing. We can conclude that in this region the upper bound for the boundary curve gives the exact boundary. We do not have a similar result for $\alpha > 0$, however in this region the curve is bounded between the canonical hyperbola and the upper bound, which approach each other as $\alpha \to \infty$.

[1] D. Dubin, J. Kiukas, J.-P. PellonPää, and K. Ylinen, (2014).