Quantum Inequalities in Quantum Mechanics

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Abstract. We study a phenomenon occurring in various areas of quantum physics, in which an observable density (such as an energy density) which is classically pointwise nonnegative may assume arbitrarily negative expectation values after quantisation, even though the spatially integrated density remains nonnegative. Two prominent examples which have previously been studied are the energy density (in quantum field theory) and the probability flux of rightwards-moving particles (in quantum mechanics). However, in the quantum field context, it has been shown that the magnitude and space-time extension of negative energy densities are not arbitrary, but restricted by relations which have come to be known as ‘quantum inequalities’. In the present work, we explore the extent to which such quantum inequalities hold for typical quantum mechanical systems. We derive quantum inequalities of two types. The first are ‘kinematical’ quantum inequalities where spatially averaged densities are shown to be bounded below. Specifically, we obtain such kinematical quantum inequalities for the current density in one spatial dimension (imposing constraints on the backflow phenomenon) and for the densities arising in Weyl–Wigner quantization. The latter quantum inequalities are direct consequences of sharp Gårding inequalities. The second type are ‘dynamical’ quantum inequalities where one obtains bounds from below on temporally averaged densities. We derive such quantum inequalities in the case of the energy density in general quantum mechanical systems having suitable decay properties on the negative spectral axis of the total energy.

Furthermore, we obtain explicit numerical values for the quantum inequalities on the one-dimensional current density, using various spatial averaging weight functions. We also improve the numerical value of the related ‘backflow constant’ previously investigated by Bracken and Melloy. In many cases our numerical results are controlled by rigorous error estimates.
1 Introduction

The uncertainty principle lies at the root of many of the counterintuitive features of quantum theory. Consider, for example, a quantum mechanical particle moving in one dimension, whose state is a superposition of right-moving plane waves. Although the expectation value of (any power of) its momentum is positive, nonetheless it is possible for the probability flux at, say, the origin to become negative. Thus the probability of finding the particle in the right-hand half-line can decrease!

We will return to this phenomenon, which has come to be known as backflow \cite{3, 7, 30}, in Section 2.1. Another, related, phenomenon occurs in quantum field theory. Even if one starts with a classical field theory in which energy densities (as measured by all observers) are everywhere positive,\footnote{In general relativity, one would say that the field obeyed the weak energy condition (WEC).} one finds that the renormalised energy density of the quantised field can assume negative values \cite{11} and (in all models known to date) can even be made arbitrarily negative at a given spacetime point by a suitable choice of state. For example, the energy density between Casimir plates is computed to be negative; a fact indirectly supported by experiment \cite{9}; see the recent review \cite{5} for an exhaustive list of up to date references). Various authors have suggested employing such effects to sustain exotic spacetime geometries containing wormholes \cite{31} or ‘warp drive’ bubbles \cite{2}. Such suggestions are, however, severely constrained \cite{23, 33} by the existence of bounds, known as quantum inequalities (QIs) or quantum weak energy inequalities (QWEIs) \cite{13, 14, 16, 18, 19, 20, 21, 22, 24, 34} which impose limitations on the magnitude and duration of negative energy densities. To give an example, let $\langle \rho(t) \rangle_\psi$ be the energy density of the free scalar field\footnote{Similar statements can be made for the Maxwell, Proca and Dirac fields \cite{32, 16, 15}.} measured along an inertial worldline in Minkowski space. Then, for any real-valued smooth compactly supported $g$, the averaged energy density obeys \cite{14, 17}

$$\int dt g(t)^2 \langle \rho(t) \rangle_\psi \geq - \int_0^\infty du Q(u)|\hat{g}(u)|^2$$

(1.1)

for all physically reasonable (Hadamard) states $\psi$, where $Q$ is a known function of polynomial growth.

The purpose of this paper is to apply techniques developed in the field theoretic setting to quantum mechanical problems. In so doing we wish to draw attention to a circle of ideas—including sharp Garding inequalities, dynamical stability and the QWEIs—which eventually ought to be seen in the wider context of quantisation theory.

We begin with a discussion of ‘kinematical QIs’ in Sect. 2 taking the probability flux as our main example. We develop bounds on spatially averaged fluxes which share some technical similarity with the QWEI proved by two of us for the Dirac field \cite{19} (see also \cite{15}). An important aspect of our treatment is the numerical analysis of these bounds. To some extent this is motivated by the recent observation of Marecki \cite{29} that QIs may have observational consequences in quantum optics; it is therefore important to know how sharp analytically tractable bounds are. The techniques used here may also be of independent interest, and we give a detailed account in Sect. 5. Before that, in Sect. 3 we establish a very general form of kinematical QIs arising in the Weyl–Wigner approach to quantizing classical systems (see, e.g., \cite{28} as a general reference on that approach). More
precisely, we consider the (quantized) configuration space density $\mathbb{R}^n \ni x \mapsto \langle \rho_F(x) \rangle_\psi$ for normalized wave-functions $\psi \in \mathcal{S}(\mathbb{R}^n)$ which are associated with classical observables $F$, i.e. functions on phase space $\mathbb{R}^n \times \mathbb{R}^n$, by

$$\langle \rho_F(x) \rangle_\psi = \int \frac{d^n p}{2\pi} F(x, p) W_\psi(x, p), \quad (1.2)$$

where $W_\psi$ denotes the Wigner function of $\psi$. Even if $F$ is everywhere nonnegative, the density $\langle \rho_F(x) \rangle_\psi$ may assume negative values owing to the indefinite sign of the Wigner function; in fact, we show that, under very general conditions on $F$, this quantity is unbounded above and below for arbitrary given $x$ upon varying $\psi$. Conversely, if $F$ belongs to a certain class of symbols (in the sense of microlocal analysis [26, 36]) which are of second order (or lower) in the momentum variables, and if $F$ is everywhere non-negative, then we establish a kinematical quantum inequality of the form

$$\int d^n x \chi(x) \langle \rho_F(x) \rangle_\psi \geq -C \quad (1.3)$$

with a suitable constant $C$ depending on the non-negative weight-function $\chi$, but not on the (normalized) wave-function $\psi$. This is a straightforward consequence of the sharp Gårding inequality [12, 27, 36]. The general result will be illustrated by a direct derivation of a kinematical QI for the energy density.

In Sect. 4 we focus attention on ‘dynamical’ QIs which bound temporal averages of the energy density in general quantum mechanical systems. (In fact our kinematical flux inequality may be regained as the special case, in which the evolution is the group of translations on the line.) These are conceptually much closer to the QIs which have been obtained in quantum field theory; in fact, the method we use to establish these dynamical QIs makes contact with the techniques employed in [19]. Some features of the general result will be illustrated by taking the harmonic oscillator as a concrete example. We summarise our main results in the conclusion, Sect. 6.

2 A motivating example

2.1 Probability backflow

We begin with a simple example: the motion of a quantum mechanical particle in one dimension. Some time ago, Alcock [3] pointed out the existence of rightwards-moving states (in which the velocity is positive with unit probability) but for which the probability of locating the particle in the right-hand half-line is instantaneously decreasing—a phenomenon known as probability back-flow. This phenomenon was subsequently studied in much greater detail by Bracken and Melloy [7] (see also [30]). To illustrate the idea, let us suppose the normalised state $\psi$ (as well as being square-integrable itself) has a continuous, square integrable first derivative. Then the corresponding probability flux at position $x$ is given by

$$j_\psi(x) = \frac{\text{Re} \overline{\psi(x)}(p\psi(x))}{m}, \quad (2.1)$$
where the momentum operator is, as usual, \( p = -i\hbar \frac{d}{dx} \) and the particle has mass \( m \). Now the spatial integral of the flux is

\[
\int j_\psi(x) \, dx = \frac{\text{Re} \left\langle \psi \mid p\psi \right\rangle}{m} = \frac{\langle p \rangle}{m}
\]

(2.2)

and therefore yields the expected velocity. If \( \psi \) is a normalised right-moving wave-packet, it may be written by means of the Fourier transform as a superposition of right-moving plane waves

\[
\psi(x) = \int \frac{dk}{2\pi} e^{ikx} \hat{\psi}(k)
\]

(2.3)

with \( \hat{\psi}(k) = 0 \) for \( k < 0 \), so

\[
\langle p \rangle_\psi = \int_0^\infty \frac{dk}{2\pi} \hbar k|\hat{\psi}(k)|^2 > 0
\]

(2.4)

and we see that the spatially integrated flux is positive. However this does not imply that the flux itself is everywhere non-negative. Indeed, suppose that

\[
\hat{\psi}_{k_0}(k) = \mathcal{N} \chi_{[0,k_0]}(k) \left( k\sqrt{3} - k_0 \right),
\]

(2.5)

where \( \chi_\Omega \) denotes the characteristic function of \( \Omega \) and \( \mathcal{N} = (k_0^3(2 - \sqrt{3})/(2\pi))^{-1/2} \) is a normalisation constant. One may calculate

\[
j_{\psi_{k_0}}(0) = \frac{\hbar k_0^2}{4\pi m} \left( \frac{1}{2} - \frac{1}{\sqrt{3}} \right) \sim -0.006 \frac{\hbar k_0^2}{m},
\]

(2.6)

which is not merely negative, but can clearly be made as negative as we wish by tuning \( k_0 \). Because the probability flux is negative at the origin, the probability of locating the particle in the left-hand half-line is instantaneously increasing, thereby providing an example of the backflow phenomenon mentioned above.

Backflow provides a nice illustration of the inadequacy of the phase velocity alone to predict the motion of a wavepacket. The three plots in Figure II indicate the evolution of the position probability density in time; although the packet moves to the right, the two main peaks are reshaped in such a way that net probability has passed from the right-hand half line to the left. The wavepacket is given by Eq. (2.5) at time \( t = 0 \) with \( k_0 = 5 \), \( m = 1/2 \) and \( \hbar = 1 \).

### 2.2 A quantum inequality for the flux

As we will see in Sect. III the backflow effect may be traced to the uncertainty principle. From this point of view, it is natural to seek bounds on its magnitude and extent. Bracken and Melloy [7] approached this question by showing that the probability \( P(t) \) of finding a right-moving particle in the left-hand half-line obeys

\[
P(t) \leq P(0) + \lambda,
\]

(2.7)
for all $t \geq 0$, where the dimensionless constant $\lambda$ is the largest positive eigenvalue of the equation

$$\frac{-1}{\pi} \int_0^\infty \frac{\sin(u^2 - v^2)}{u-v} \varphi(v) \, dv = \lambda \varphi(u)$$

(2.8)

(for $\varphi \in L^2(\mathbb{R}^+)$). They also presented numerical evidence that $\lambda \sim 0.04$. Using the numerical methods described in Sect. 5, we have recalculated this quantity to a much higher accuracy, although we have been unable to obtain consonant analytical error estimates.

It turns out to be convenient to change variables to $x = u^2$; we then consider the truncation of the resulting integral kernel to $\left[0, X\right]$. The maximum eigenvalue $\lambda(X)$ was then calculated for values of $X$ ranging from 6000 to 24000, using $X/2$ quadrature nodes. This choice was based on calculations using a variety of densities for values of $X$ around 2000 for which $X/2$ nodes provide accuracy to 5 significant figures. By contrast, the largest calculation conducted in [7] corresponds to $X = 625$, which reflects the increase in available computing power over the past decade. The resulting data may be fitted to a remarkable degree by the form $\lambda(X) = a + b/\sqrt{X}$ (as already noted by Bracken and Melloy for their data). Using a least squares fit to this, we obtain the estimate $\lambda = 0.03845182014$ with a maximum percentage residual error under $4 \times 10^{-4}\%$. Assuming the residual errors would be comparable for larger $X$, this suggests that $\lambda = 0.038452$ to this level of precision. Our data points and the best-fit curve are shown in Fig. 2.

One may interpret the Bracken–Melloy bound (2.7) as a demonstration of the transitory nature of backflow: large negative fluxes for right-moving states must be short-lived. Here, we present an apparently new bound, which demonstrates that such fluxes are also of small spatial extent, and whose proof is related to the quantum weak energy inequalities derived by two of us for the Dirac quantum field [19] (see also [15]). We consider spatially smeared quantities of the form

$$j_\psi(f) = \int j_\psi(x) f(x) \, dx,$$

(2.9)

which may be regarded as the instantaneous probability flux measured by a spatially extended detector. For any smooth, compactly supported, complex-valued function $g$, we
will show that
\[ \int j_\psi(x) |g(x)|^2 \, dx \geq -\frac{\hbar}{8\pi m} \int dx |g'(x)|^2 \] (2.10)
for all normalised states \( \psi \) belonging to the class \( \mathcal{R} \) of right-moving states defined by
\[ \mathcal{R} = \{ \psi \in L^2(\mathbb{R}) : \hat{\psi}(k) = 0 \text{ for } k < 0 \text{ and } \psi' \text{ continuous and square-integrable} \} . \] (2.11)

In fact, the conditions on both \( g \) and \( \psi \) may be weakened slightly.\(^3\)

Before giving the proof, let us make three observations.

1. First, we note that there is no upper bound on the smeared flux. To see this, choose any normalised \( \psi \in \mathcal{R} \) and let \( \psi_\lambda(x) = e^{i\lambda x} \psi(x) \). We have \( \psi_\lambda \in \mathcal{R} \) for \( \lambda \geq 0 \); moreover,
\[
\hat{j}_{\psi_\lambda}(x) = \hat{j}_\psi(x) + \frac{\lambda \hbar}{m} |\psi(x)|^2
\] (2.12)
so \( \int j_\psi(x)f(x) \, dx \to +\infty \) as \( \lambda \to +\infty \).

2. Second, the scaling behaviour of the above bound may be investigated by replacing \( g \) by \( g_\lambda(x) = \lambda^{-1/2} g(x/\lambda) \), whereupon the right-hand side of inequality (2.10) scales

\[^3\text{In particular, continuity of } \psi' \text{ may be weakened to } \psi \in AC(\mathbb{R}) \cap L^2(\mathbb{R}) \text{ with } \psi' \in L^2(\mathbb{R}) \text{ at the expense of augmenting some statements with the qualification 'almost everywhere'; by an approximation argument it is easy to see that (2.10) holds for all } g \text{ belonging to the Sobolev space } W^{1,2}(\mathbb{R}).\]
by a factor of $\lambda^{-2}$. The limit $\lambda \to 0$ corresponds to the unboundedness below of the probability flux at a point, while the limit $\lambda \to \infty$ is consistent with the fact that $\langle p \rangle_\psi \geq 0$ for $\psi \in \mathcal{R}$ (because the bound vanishes more rapidly than $\lambda^{-1}$). Roughly speaking, our bound asserts that the magnitude of negative flux times the square of its spatial extent satisfies a state-independent upper bound on $\mathcal{R}$. Thus the extent of backflow is limited both in space and in time.

Note also that the bound (2.10) vanishes in both the classical limit $\hbar \to 0$ and the limit of large mass. This differs from Bracken and Melloy’s inequality (2.7) in which the dimensionless constant $\lambda$ is independent of $\hbar$ and $m$.

We remark that—again in contrast to [7]—our result is kinematical rather than dynamical: no specific Hamiltonian is invoked. Here, ‘kinematic’ refers to the kinematics of the Schrödinger representation, i.e., the (unique) regular representation of the Heisenberg commutation relations.

3. Finally, on integration by parts, Eq. (2.10) can be reformulated as the assertion that for each normalised $\psi \in \mathcal{R}$, the Schrödinger operator

$$H_\psi = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + 4\pi \hbar j_\psi(x)$$

(2.13)

is positive on the space of smooth compactly supported functions $g$, in the sense that

$$\int g(x)(H_\psi g)(x) \geq 0$$

(2.14)

for all such $g$. Although the physical significance of this reformulation is not clear, it can provide useful necessary conditions for a given function $j(x)$ to be the flux of a right-moving state. Only if the corresponding Schrödinger operator has no bound states can this be the case. This can be sharpened slightly: as an illustration, suppose $j_\psi(x)$ is the flux of a state in $\mathcal{R}$ with $j_\psi(x) \leq -M$ on some open interval $I$ of length $a$. Then positivity of $H_\psi$ on $C_0^\infty(I)$ implies that the Friedrichs extension $H_M$ of the operator

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - 4\pi \hbar M$$

on $C_0^\infty(I) \subset L^2(I)$

(2.15)

is also positive. Since the Friedrichs extension of this operator corresponds to the imposition of Dirichlet boundary conditions at the boundary of $I$, $H_M$ has spectrum

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} - 4\pi \hbar M \quad (n = 1, 2, 3, \ldots)$$

(2.16)

so we deduce (from $E_1 \geq 0$) that $M \leq \hbar \pi/(8ma^2)$. This provides a more quantitative version of the connection between the magnitude and spatial extent of negative fluxes. Similar ideas have been employed in the context of quantum weak energy inequalities [18] to cast light on the ‘quantum interest conjecture’ of Ford and Roman [25].
We now establish the quantum inequality (2.10). It is sufficient to prove this for the case in which \(g \in C_0^\infty(\mathbb{R})\) is real-valued. Setting \(f(x) = g(x)^2\) and writing \(M_f\) for the multiplication operator \((M_f \psi)(x) = f(x)\psi(x)\), we have

\[
\int j_\psi(x)f(x)\,dx = \frac{1}{m} \text{Re} \langle \psi \mid M_f p \psi \rangle
\]

where we have used the fact that \(\text{Re} \langle \psi \mid M_g [M_g, p] \psi \rangle = 0\). We therefore may obtain a bound by estimating the portion of this integral arising from \(k < 0\):

\[
\int j_\psi(x)f(x)\,dx \geq \frac{\hbar}{m} \int_{-\infty}^0 \frac{dk}{2\pi} k |\hat{M}_g \psi(k)|^2 = -\frac{\hbar}{m} \int_0^\infty \frac{dk}{2\pi} k |\hat{M}_g \psi(-k)|^2. \tag{2.18}
\]

By the convolution theorem

\[
\hat{M}_g \psi(k) = \int_0^\infty \frac{dk'}{2\pi} \hat{\psi}(k') \hat{g}(k-k'), \tag{2.19}
\]

where the restriction to \(k' \in \mathbb{R}^+\) is permissible for \(\psi \in \mathcal{B}\). Now a straightforward application of Cauchy-Schwarz gives

\[
|\hat{M}_g \psi(-k)|^2 \leq \int_0^\infty \frac{dk'}{2\pi} |\hat{g}(k+k')|^2, \tag{2.20}
\]

where we have also used \(|\hat{g}(-k)|^2 = |\hat{g}(k)|^2\) (since \(g\) is real) and \(||\psi\|| = 1\). Substituting in (2.18), we now calculate

\[
\int j_\psi(x)f(x)\,dx \geq -\frac{\hbar}{m} \int_0^\infty \frac{du}{2\pi} \int_0^\infty \frac{du}{2\pi} u^2 |\hat{g}(u)|^2 \int_0^u dk \]

where we have changed variables from \((k, k')\) to \((u, k)\) with \(u = k + k'\), used evenness of \(|\hat{g}(u)|\) and Parseval’s theorem. This completes the proof of the quantum inequality (2.10).
The later stages of this argument may be rephrased as follows. The inequality (2.18) asserts that
\[ \int j_\psi(x)f(x) \, dx \geq -\frac{\hbar}{m} \| T \hat{\psi} \|^2 \] (2.22)
where the operator \( T \) acts on \( L^2(\mathbb{R}^+, dk/(2\pi)) \) by
\[ (T\varphi)(k) = \int \frac{dk'}{2\pi} \sqrt{k} \hat{g}(-k - k') \varphi(k') \] (2.23)
and is easily seen to be Hilbert–Schmidt. Varying over normalised \( \psi \), the right-hand side of Eq. (2.22) is bounded below by \( -\| T \|^2 \), where \( \| T \| \) denotes the operator norm of \( T \). This leads to the bounds
\[ \int j_\psi(x)f(x) \, dx \geq -\frac{\hbar}{m} \| T \|^2 \geq -\frac{\hbar}{m} \| T \|_{\text{H.S.}}^2, \] (2.24)
where the last inequality holds because the Hilbert–Schmidt norm \( \| T \|_{\text{H.S.}} \) dominates the operator norm. The calculation in (2.21) in fact precisely computes this final bound.

To summarise, we have seen that, even for a right-moving state \( \psi \in \mathcal{R} \), the flux \( j_\psi \) need not be pointwise nonnegative; moreover by tuning the state, one may arrange the normalised flux \( j_\psi(x) \) to be as negative as one likes at a given fixed \( x \). However, weighted spatial averages of the flux are bounded below in terms of the weight function alone. This condition may be reformulated as asserting the positivity of the Hamiltonian for a particle moving in a potential given (up to constants) by the probability flux of any state in \( \mathcal{R} \).

### 2.3 Numerical results and sharper bounds

We illustrate our bound by reference to four weight functions: a Gaussian, a squared Lorentzian and two compactly supported weights which we call the truncated cosine and the smoothed truncated cosine. (Neither of the compactly supported weights are \( C^\infty \), but they have sufficient smoothness for the above argument to hold; see footnote 3 above.) Our weight functions are summarised in Table 1 along with the corresponding bound arising from Eq. (2.10). In each case, \( f_\lambda \) has unit integral, the parameter \( \lambda \) controls the sampling width and \( g_\lambda(x) = \sqrt{f_\lambda(x)} \). For later reference we have also given the Fourier transforms of \( f_\lambda \) and \( g_\lambda \).

We wish to compare the above bound with two sharper (but less analytically tractable) bounds: the bound arising from the first inequality in (2.24) and a direct numerical estimate of the infimum of the integrated flux. In the first case, we are required to find the operator norm of \( T \). Our numerical approach proceeds by first truncating the kernel to an interval \([0, K]\)—we are able to estimate the error incurred here by using bounds obtained from the Hilbert–Schmidt norm—and applying a numerical quadrature scheme due originally to Fredholm (see e.g., Sec. 4.1 of [4] or Chapter 4 of [10]) to the truncated kernel. This leads to a matrix whose eigenvalues approximate those of the truncated kernel and hence the original operator, and which can be computed using standard numerical packages. Full details, including a discussion of error estimates, are given in Sect. 5. This leads to quantum inequalities
\[ \int j_\psi(x)f_\lambda(x) \, dx \geq -\frac{\hbar C}{m\lambda^2}, \] (2.25)
| $f_\lambda$ | $(\lambda \sqrt{\pi})^{-1}e^{-(x/\lambda)^2}$ | $2\lambda^3\pi^{-1}/(x^2 + \lambda^2)^2$ | $\theta(\lambda - |x|)/\lambda \cos(x\pi/(2\lambda))$ | $4\theta(\lambda - |x|)/(3\lambda) \cos(x\pi/(2\lambda))^4$ |
| $\hat{f}_\lambda$ | $e^{-(\lambda u)^2/4}$ | $(1 + \lambda |k|)e^{-\lambda |k|}$ | $\pi^2 \sin(\lambda k)$ | $\frac{\pi^4 \sin(\lambda k)}{\lambda k(\pi^2 - k^2 \lambda^2)}$ |
| $\hat{g}_\lambda$ | $\sqrt{2\lambda \pi^{1/4}}e^{-(u\lambda)^2/2}$ | $\sqrt{2\lambda \pi}e^{-\lambda |k|}$ | $4\pi \sqrt{\lambda \cos(\lambda k)}$ | $\frac{2\pi^2 \sin(\lambda k)}{k \sqrt{3\lambda(\pi^2 - k^2 \lambda^2)}}$ |
| QI bound | $-\hbar/(16\pi m \lambda^2)$ | $-\hbar/(16\pi m \lambda^2)$ | $-\hbar/(32m \lambda^2)$ | $-\hbar/(24m \lambda^2)$ |
| $\approx \hbar/(m \lambda^2 \times)$ | $-0.01989436788$ | $-0.01989436788$ | $-0.09817477044$ | $-0.1308996939$ |

Table 1: Compendium of sampling functions considered.

| Gaussian | Squared Lorentzian | Truncated cosine | Smoothed truncated cosine |
|----------|--------------------|------------------|--------------------------|
| $K$      | $\mu(K)$          | $K$              | $\mu(K)$                 | $K$              | $\mu(K)$                 |
| 10       | -0.0048295212087  | 30               | -0.002980544308          | 2000             | -0.029012801924          |
| 20       | -0.0048295668511  | 40               | -0.029012804495          | 140              | -0.036095566956          |
| 30       | -0.0048295668517  | 50               | 2200                     | -0.029012806174  |
| 40       | 60                | 2600             | -0.029012807318          | 160              | -0.036095567038          |
| 50       | 70                | 2800             | -0.029012808114          | 180              | -0.036095567056          |
| 60       | 80                | 3000             | -0.029012808686          | 200              | -0.036095567060          |

Table 2: Numerical estimation of $\inf \sigma(J)$ for various kernels.
where the constant $C$ depends on the particular weight function used and is given:

| Kernel               | $C$           | Accuracy | Improvement |
|----------------------|---------------|----------|-------------|
| Gaussian             | 0.01958128485 | 10 S.F.  | 1.6%        |
| Squared Lorentzian   | $(16\pi)^{-1}$| Exact    | 0           |
| Trunc. cosine        | 0.08463957004 | 2 S.F.?  | 16%         |
| Smooth trunc. cosine | 0.125047838   | At least 3 S.F. | 4.5% |

Note that we were only able to obtain fairly weak error bounds in the truncated cosine case. In each case, the improvement on the analytical bound is relatively small. We may interpret these results as showing that $T = R + S$ where $R$ has rank 1 and the Hilbert–Schmidt norm of $S$ is small relative to that of $T$. This is most apparent in the squared Lorentzian case, in which $T$ is itself exactly rank 1 and no improvement is obtained by using the operator norm. It would be interesting to understand the origin of this apparently general phenomenon.

Our second numerical calculation aims to compute the infimum of the spectrum of the unbounded integral operator

\[
(J \varphi)(k) = \frac{\hbar}{2} \int_0^\infty \frac{dk'}{2\pi} (k + k') \hat{f}_\lambda(k - k') \varphi(k').
\]  

(2.26)

We proceed by truncating the kernel to the interval $[0, K]$, computing the minimum eigenvalue $\mu(K)$ using sufficiently many quadrature points to obtain machine precision. We then increase $K$ until convergence of $\mu(K)$ is obtained, again to machine precision. Our results are given in Table 2, in which we give $\mu(K)$ in units of $\hbar/(m\lambda^2)$. Blank entries indicate that the computed value was identical to the last printed number in that column. The density of quadrature points used (per unit $K$) was 5 for the Gaussian, 1 for the truncated cosine, and 5 for the smoothed truncated cosine, although higher densities were also used as a numerical check (40, 2, and 10 respectively). The results for the squared Lorentzian were rather slower to converge as the density increased (perhaps because the kernel fails to be everywhere smooth) and were computed using a density of 60. For $K < 80$, a density of 70 was used as a check.

To summarise, we have seen that a) the limitations of our flux QI do not lie in the estimation of an operator norm by a Hilbert–Schmidt norm, but rather in the earlier stages of the derivation (probably the estimate (2.18)); b) the overall scope for improvement on our flux QI is roughly a factor of between 3 and 7 (in our examples), and it is clear that the sharp bound is not simply a multiple of our bound (2.10) (in contrast to the situation for two-dimensional massless quantum fields [21, 14]).

3 The Wigner function and Kinematical Quantum Inequalities

It is worth emphasising that phenomena similar to those presented above arise naturally in the context of Weyl quantisation, in which the phase space aspect of quantum mechanics is brought to the fore. In our discussion we will consider the phase space to be $\mathbb{R}^n \times \mathbb{R}^n$.
(see, e.g., [28] for Weyl quantisation on manifolds). We recall that the central object in this approach is the Wigner function \( W_\psi \) defined on phase space by

\[
W_\psi(x, p) = \left( \frac{2}{\hbar} \right)^n \int d^ny e^{2ipy/\hbar} \psi(x+y)\psi(x-y),
\]

where \( \psi \in L^2(\mathbb{R}^n) \) is the corresponding normalised quantum mechanical state vector. The classical analogue of \( W_\psi(x, p) \) would be a probability distribution on phase space; as is well known, however, \( W_\psi \) is not itself a probability distribution because it is not guaranteed to be everywhere nonnegative. This has important consequences for observables obtained via Weyl quantisation, which proceeds as follows.

Given an observable on the classical phase space, i.e., a smooth function \( F : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R} \), Weyl quantisation defines an operator \( F_w \) whose expectation values are given (for normalised \( \psi \)) by

\[
\langle F_w \rangle_\psi = \int \frac{d^nxd^np}{(2\pi)^n} F(x, p) W_\psi(x, p).
\]

The action of this operator may be written in the form

\[
(F_w \psi)(x) = \int \frac{d^nyd^np}{(2\pi\hbar)^n} F([x + y]/2, p) e^{i(x-y)\cdot p/\hbar} \psi(y).
\]

Let us note that this procedure also yields a natural definition for the quantum mechanical density associated with a classical observable. Namely, setting

\[
\langle \rho_F(x) \rangle_\psi = \int \frac{d^np}{(2\pi)^n} F(x, p) W_\psi(x, p),
\]

it is clear that the spatial integral of \( \langle \rho_F(x) \rangle_\psi \) yields the expectation value \( \langle F_w \rangle_\psi \) for all \( F \) and \( \psi \) (modulo domain questions\(^5\)).

Now, because the Wigner function need not be everywhere positive, we see that the Weyl quantisation of a nonnegative classical observable may assume negative expectation values. This situation is exacerbated for the densities defined above (see statement (II) below). However, we will show that kinematical quantum inequalities may be derived, under certain conditions. Indeed, these bounds are obtained as applications of the so-called sharp Gårding inequalities in the theory of pseudodifferential operators [36, 12, 27]. It is interesting to note that Fefferman and Phong, to whom the most general sharp Gårding results are due, were guided by intuition arising from quantum mechanics: in particular, the uncertainty principle.

We begin by specifying more precisely the class of classical observables. For \( m \in \mathbb{N} \), the symbol class \( S^m \) (often denoted more precisely as \( S^m_{1,0} \)) is defined to be the set of smooth functions \( F : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{C} \) such that, for each compact \( K \subset \mathbb{R}^n \) and \( n \)-dimensional multi-indices \( \alpha, \beta \), there exists a constant \( C_{K, \alpha, \beta} \) such that

\[
|\langle D_x^\alpha D_p^\beta F \rangle(x, p)| \leq C_{K, \alpha, \beta}(1 + |p|)^{m-|\beta|}
\]

\(^4\)Precise growth conditions will be specified below.

\(^5\)For example, this will certainly hold for \( F \) of polynomially bounded growth and \( \psi \) belonging to the Schwartz class.
for all \((x,p) \in K \times \mathbb{R}^n\) (see, e.g., [26, 36] for multi-index notation). By \(S^m_{\text{hom}}\), we denote the set of \(F \in S^m\) admitting a (unique) decomposition \(F = F_{\text{pr}} + F_{\text{sub}}\) such that the principal symbol \(F_{\text{pr}}\) belongs to \(S^m\), is homogeneous of degree \(m\) in momentum, i.e., \(F_{\text{pr}}(x, \lambda p) = \lambda^m F_{\text{pr}}(x, p)\) for all \((x, p) \in \mathbb{R}^n\) and \(\lambda \in \mathbb{R}\), and is nonzero except at vanishing momentum, while the sub-principal symbol \(F_{\text{sub}}\) belongs to \(S^{m-1}\).

For \(F \in S^m\), the Weyl quantisation \(F_w\) is a continuous linear map from \(C_0^\infty(\mathbb{R}^n)\) to \(C^\infty(\mathbb{R}^n)\), so Eq. (3.2) holds for all normalised \(\psi \in C_0^\infty(\mathbb{R}^n)\). The density \(\langle \rho_F(x) \rangle_\psi\) is in fact defined (and indeed smooth in \(x\)) for all \(\psi\) belonging to the Schwartz class \(\mathcal{S}(\mathbb{R}^n)\); however, it is only guaranteed to be integrable for \(\psi \in C_0^\infty(\mathbb{R}^n)\).

Below, we will establish the following observations:

(I) Suppose \(F \in S^m_{\text{hom}}\) is real, for some \(m \geq 1\). Then, for each \(x\), the density \(\langle \rho_F(x) \rangle_\psi\) is unbounded from below and below as \(\psi\) varies in \(C_0^\infty(\mathbb{R}^n)\) with \(||\psi||_{L^2} = 1\).

(II) Suppose \(F \in S^2\) is nonnegative, \(F(x, p) \geq 0\) for all \((x, p)\) and let \(\chi \in C_0^\infty(\mathbb{R}^n)\) be nonnegative. Then there exists a constant \(C \geq 0\), depending on \(F\) and \(\chi\), such that

\[
\int d^n x \chi(x) \langle \rho_F(x) \rangle_\psi \geq -C
\]  

for all \(\psi \in \mathcal{S}(\mathbb{R}^n)\) with \(||\psi||_{L^2} = 1\).

To establish (I) we may assume without loss of generality that \(x = 0\), for which we have

\[
\langle \rho_F(0) \rangle_\psi = \left(\frac{2}{\hbar}\right)^n \int \frac{d^np \, d^ny}{(2\pi)^n} F(0, p) \overline{\psi(y)} \psi(-y)
\]

for normalised \(\psi \in C_0^\infty(\mathbb{R}^n)\). Setting \(\psi_\lambda(x) = \lambda^{-n/2} \psi(x/\lambda), \ (\lambda > 0)\) and making the obvious change of variables,

\[
\langle \rho_F(0) \rangle_{\psi_\lambda} = \left(\frac{2}{\lambda \hbar}\right)^n \int \frac{d^np \, d^ny}{(2\pi)^n} F(0, p/\lambda) \overline{\psi(y)} \psi(-y)
\]

so, bearing in mind that

\[
|F(0, p/\lambda) - F_{\text{pr}}(0, p/\lambda)| \leq C(1 + |p/\lambda|)^{m-1}
\]

by definition of \(S^m_{\text{hom}}\) and Eq. (3.5), we obtain

\[
\lambda^{m+n} \langle \rho_F(0) \rangle_{\psi_\lambda} \longrightarrow \left(\frac{2}{\hbar}\right)^n \int \frac{d^np \, d^ny}{(2\pi)^n} F_{\text{pr}}(0, p) \overline{\psi(y)} \psi(-y)
\]

as \(\lambda \to 0^+\). It now remains to show that the right-hand side of this expression attains values of both signs as \(\psi\) varies in \(C_0^\infty(\mathbb{R}^n)\). To this end, assume (without loss) that \(F_{\text{pr}}(0, p)\) depends nontrivially on the first coordinate, \(p_1\), of \(p\). Integrating by parts, the right-hand side of (3.10) in the form \(P_y(\psi(y) \psi(-y))|_{y=0}\), where \(P_y\) is a homogeneous linear partial differential operator (in \(y\)) of order \(m\) with (possibly complex) constant coefficients \(c_{\alpha}\). We now consider \(\psi\) of the form

\[
\psi(y) = f(y_1) e^{i(y_2 + \cdots + y_n)} \chi(y)
\]  

(3.11)
where $\chi \in C_0^\infty(\mathbb{R}^n)$ is equal to unity in a neighbourhood of the origin and $f \in C_0^\infty(\mathbb{R})$. For such $\psi$ we have

$$P_y(\overline{\psi(y)}\psi(-y))|_{y=0} = Q_{y_1}(\overline{f(y_1)}f(-y_1))|_{y_1=0}$$

for some ordinary differential operator

$$Q_{y_1} = \sum_{k=0}^q c_k (-i)^k \frac{q^k}{dy_1^k}$$

of order $1 \leq q \leq m$ with constant real coefficients. (That $Q_{y_1}$ is of order at least one is a consequence of our assumption that $F_{pr}(0, p)$ depends nontrivially on $p_1$; reality of the $c_k$ holds because the right-hand side of Eq. (3.10) is manifestly real for all $\psi \in C_0^\infty(\mathbb{R}^n)$.) We now choose $f$ so that $f(0) = 1$ and $f^{(k)}(0) = 0$ for $1 \leq k \leq q - 1$. Then by Leibniz’ formula,

$$P_y(\overline{\psi(y)}\psi(-y))|_{y=0} = c_q (-i)^q \left( f^{(q)}(0) + (-1)^q f^{(0)}(0) \right) + c_0.$$  

It is now obvious that $f$ may be chosen so that the right-hand side of this expression adopts values of both signs, completing the argument.

Statement (II) is straightforward: because $\chi \in C_0^\infty(\mathbb{R}^n)$ and $F \in S_2$, the symbol $\chi F$ obeys uniform bounds

$$|\langle D_{x}^{\alpha} D_{p}^{\beta} \chi F(x, p) \rangle| \leq C_{\alpha, \beta} (1 + |p|)^{m-|\beta|}$$

for all $(x, p) \in \mathbb{R}^n \times \mathbb{R}^n$, so the sharp Gårding inequality (Corollary 18.6.11 in [27] with $\delta = 0$, $\rho = 1$; see also Eq. (18.1.1)’ therein) entails the existence of a constant $C$ such that

$$\int d^n x \chi(x) \langle \rho_F(x) \rangle_\psi = \langle (\chi F)_w \rangle_\psi \geq -C$$

for all normalised $\psi \in \mathcal{S}(\mathbb{R}^n)$. This is the required kinematical quantum inequality.

We now give two examples to illustrate the above ideas.

**Example 1:** Consider a classical Hamiltonian

$$H(x, p) = \frac{p^2}{2m} + V(x)$$

on $\mathbb{R}^n \times \mathbb{R}^n$ with $V \in C^\infty(\mathbb{R}^n)$. The Hamiltonian density obtained from Eq. (3.4) is

$$\langle \rho_H(x) \rangle_\psi = \frac{\hbar^2}{4m} \left( |\nabla \psi(x)|^2 - \text{Re} \overline{\psi(x)}(\Delta \psi)(x) \right) + V(x)|\psi(x)|^2,$$

where $\Delta = \nabla^2$ is the Laplacian. Clearly $\langle \rho_H(x) \rangle_\psi$ may be made arbitrarily negative as $\psi$ varies in $C_0^\infty(\mathbb{R}^n)$ by arranging that $\nabla \psi(x) = 0$, $\overline{\psi(x)}\Delta \psi(x) > 0$ and then—as in (I) above—scaling $\psi$ about $x$, introducing

$$\psi_\lambda(y) = \lambda^{-n/2} \psi((y - x)/\lambda)$$
for which
\[ \langle \rho_H(x) \rangle_{\psi_{\lambda}} = -\lambda^{-(n+2)} \frac{\hbar^2}{4m} \text{Re} \bar{\psi}(x)(\Delta \psi)(x) + \lambda^{-n} V(x)|\psi(x)|^2. \] (3.20)

As in the proof of (I), the subprincipal symbol drops out in the limit \( \lambda \to 0^+ \), so
\[ \langle \rho_H(x) \rangle_{\psi_{\lambda}} \to -\infty. \]

Since \( H \in S^2 \) we already know that a kinematical quantum inequality exists. However, it is instructive to give a direct argument for this, which also yields an explicit bound. To this end, we note that, for any nonnegative \( \chi \in C^\infty_0(\mathbb{R}^n) \) and normalised \( \psi \in \mathcal{S}(\mathbb{R}^n) \),
\[
\int d^n x \chi(x) \langle \rho_H(x) \rangle_{\psi} = \frac{1}{4m} \langle p_i \psi | M_\chi p_i \psi \rangle + \frac{1}{8m} \langle \psi | (M_\chi p^2 + p^2 M_\chi) \psi \rangle + \langle \psi | M_{\chi V} \psi \rangle
\] (3.21)
where \( p_i = -i\hbar \nabla_i \) and \( (M_f \psi)(x) = f(x)\psi(x) \) is the operator of multiplication by \( f \). Now \([M_\chi, p_i] = i\hbar M_{\nabla_i \chi} \), so
\[
M_\chi p^2 + p^2 M_\chi = 2p_i M_\chi p_i + i\hbar [M_{\nabla_i \chi}, p_i] = 2p_i M_\chi p_i - \hbar^2 M_{\Delta \chi}
\] (3.22)
and hence
\[
\int d^n x \chi(x) \langle \rho_H(x) \rangle_{\psi} = \frac{1}{2m} \langle p_i \psi | M_\chi p_i \psi \rangle + \langle \psi | M_L \psi \rangle
\] (3.23)
where
\[
L(x) = -\frac{\hbar^2}{8m}(\Delta \chi)(x) + V(x)\chi(x).
\] (3.24)
Since the first term in (3.23) is nonnegative, we obtain the quantum inequality
\[
\int d^n x \chi(x) \langle \rho_H(x) \rangle_{\psi} \geq \inf_{x \in \mathbb{R}^n} \left( -\frac{\hbar^2}{8m}(\Delta \chi)(x) + V(x)\chi(x) \right).
\] (3.25)
for all nonnegative \( \chi \in C^\infty_0(\mathbb{R}^n) \) and \( \psi \in \mathcal{S}(\mathbb{R}^n) \). We note as a curiosity the appearance of a Schrödinger operator applied to the weight \( \chi \) (rather than the state \( \psi \)). In the case of a nonnegative potential, we may obtain a QI (slightly weaker than that given above) in the form
\[
\int d^n x \chi(x) \langle \rho_H(x) \rangle_{\psi} \geq \frac{1}{4} \inf_{x \in \mathbb{R}^n} (H\chi)(x).
\] (3.26)

**Example 2:** We now show that (II) allows us to deduce the existence of a kinematical flux QI on rightwards moving states. Let \( f \) be a nonnegative smooth compactly supported function. The averaged probability flux \( j_\psi(f) \) is easily seen to be the expectation in state \( \psi \) of the Weyl quantisation \( j(f) \) of \( f(x)p/m \), which is a (first order) element of the symbol class \( S^2 \) (but is of course negative for \( p < 0 \)). Now let \( \eta(p) \) be smooth, vanishing for \( p < 0 \) and equal to \( p \) for \( p \) greater than some \( p_0 \), and set \( F(x, p) = f(x)\eta(p)/m \). Then the quantisation \( F_w \) differs from \( j(f) \) on \( \mathcal{B} \cap \mathcal{S}(\mathbb{R}) \) only by a bounded operator. Accordingly (II) entails that \( j_\psi(f) \) is bounded below for normalised \( \psi \in \mathcal{B} \cap \mathcal{S}(\mathbb{R}) \). Of course, this argument does not determine the magnitude of the bound, in contrast to the direct approach of Sect. 2.2.
We should like to remark that in [6] there appears a result which is complementary to ours; in that reference, the authors consider the one-dimensional case $n = 1$ and show that there is a $\psi$-independent bound below (and above) on the integral of the Wigner function over elliptic sub-regions of the phase-plane which is much sharper than that implied by the a priori uniform bounds on the Wigner function. This is again an effect of averaging, this time over a region of finite extension in both $x$- and $p$-space. It would be interesting to see if this result can be generalized to higher dimensions through a generalization of (II) to a more general class of symbols; however, it is not at all clear that this can be accomplished as it apparently goes beyond the scope of sharp Gårding inequalities.

4 Dynamical quantum inequalities

In this section we turn to a different type of QI, which is closer to those studied in quantum field theory. The focus here is on time-averages of the energy density at a fixed spatial point: we will refer to the QI bounds obtained as dynamical quantum inequalities. To keep the discussion fairly general, we assume that configuration space $M$ is a topological space carrying a measure $\nu$, so that the state space is $\mathcal{H} = L^2(M, d\nu)$. The dynamics is assumed to be generated by a self-adjoint Hamiltonian $H$ which is defined on a dense domain in $\mathcal{H}$. Each normalised state $\psi$ belonging to the domain of $H$ then determines both a position probability density $\langle \rho(t,x) \rangle_\psi$ and a Hamiltonian density $\langle h(t,x) \rangle_\psi$ by

$$\langle \rho(t,x) \rangle_\psi = |\psi_t(x)|^2 \quad (4.1)$$
$$\langle h(t,x) \rangle_\psi = \text{Re} \psi_t(x)(H\psi_t)(x) \quad (4.2)$$

where $\psi_t = e^{-iHt/\hbar}\psi$. This definition of the energy density differs from that employed in Sect. [3] note that we are not assuming in this section that $H$ is the quantisation of a classical observable, in which case the above would appear to be the most natural definition. In particular, both the quantities defined are integrable with respect to the measure $d\nu(x)$ for each $t \in \mathbb{R}$, with integrals equal to unity and $\langle H \rangle_\psi$ respectively. However, we will be interested mainly in time averages of these quantities at some fixed point $x \in M$. In so doing, we immediately encounter the problem that it does not generally make sense to speak of the value of an $L^1$-function at a point.\footnote{Elements of the space $L^1(M, d\mu)$ are really equivalence classes of functions agreeing almost everywhere.} To avoid this, we introduce the spaces $\mathcal{H}_k = D((1 + H^2)^{k/2})$ and assume that, for some $k > 0$, each element in $\mathcal{H}_k$ should be (almost everywhere equal to) a continuous function and that for each $x \in M$ there is a vector $\eta_x \in \mathcal{H}$ such that

$$\psi(x) = \langle \eta_x | p_k(H)\psi \rangle \quad \forall \psi \in \mathcal{H}_k. \quad (4.3)$$

Here, $\psi(x)$ means the value at $x$ of the continuous function to which $\psi$ is almost everywhere equal, and we have written $p_k(E) = (1 + E^2)^{k/2}$. Therefore, the functional $\psi \mapsto \langle \eta_x | p_k(H)\psi \rangle$ on $\mathcal{H}_k$ coincides with the $\delta$-distribution concentrated at $x$, so that formally [as it is not an element of $\mathcal{H}$] $p_k(H)^*\eta_x$ is the $\delta$-distribution. In practice, these
assumptions are fairly mild: in particular, for the case in which \( H \) is minus the Laplacian on some manifold they are simply a transcription of the content of Sobolev’s lemma. We remark that the necessary regularity in quantum field theoretic quantum inequalities is obtained by restricting to the class of Hadamard states, which would correspond to \( \mathcal{H}_\infty = \bigcap_{k \in \mathbb{N}} \mathcal{H}_k \) in the present context.

It now makes sense to define the position and Hamiltonian densities as
\[
\langle \rho(t, x) \rangle_\psi = \langle \eta_x \mid p(H) \psi \rangle^2 \\
\langle h(t, x) \rangle_\psi = \text{Re} \langle p(H) \psi \mid \eta_x \rangle \langle \eta_x \mid p_k(H) H \psi \rangle
\]
for normalised states \( \psi \in \mathcal{H}_{k+1} \). Furthermore, one may easily check (using Cauchy-Schwarz) that these quantities are bounded in \( t \), so the time-averaged quantities \( \langle \rho_x(f) \rangle_\psi \) and \( \langle h_x(f) \rangle_\psi \) given by
\[
\langle \rho_x(f) \rangle_\psi = \int dt f(t) \langle \rho(t, x) \rangle_\psi
\]
and the analogous equation for \( \langle h_x(f) \rangle_\psi \) are well-defined for any smooth compactly supported function \( f \).

From now on, we denote the spectral measure of \( H \) by \( dP_E \). (In the case where \( H \) may be diagonalised by a basis of orthogonal eigenvectors \( \phi_n \) with simple eigenvalues \( E_n \),
\[
\int d\langle \psi \mid P_E \varphi \rangle f(E) = \sum_n \langle \psi \mid \phi_n \rangle \langle \phi_n \mid \varphi \rangle f(E_n)
\]
\[
= \int dE \sum_n \delta(E - E_n) \langle \psi \mid \phi_n \rangle \langle \phi_n \mid \varphi \rangle f(E);
\]
more generally, the projection-valued measure allows for the case of varying—even infinite—multiplicities and for both continuous and discrete spectrum.) While there is some ambiguity in choosing \( k \) and \( \eta_x \) such that Eq. \( 4.3 \) holds, the measure on \( \mathbb{R} \) defined by
\[
\mu_x(\Delta) = \int_{\Delta} \langle \eta_x \mid dP_E \eta_x \rangle p_k(E)^2
\]
for bounded Borel sets \( \Delta \) has an independent meaning. In fact, \( \mu_x(\Delta) \) is simply the diagonal \( P_\Delta(x, x) \) of the integral kernel of the spectral projection \( P_\Delta \) of \( H \) on \( \Delta \),\(^7\) given by
\[
\mu_x(\Delta) = \sum_{n : E_n \in \Delta} |\phi_n(x)|^2,
\]
if \( H \) has purely discrete spectrum. Below, it will occasionally be useful to consider the corresponding measure arising from self-adjoint operators other than \( H \); in these cases, we will write \( \mu_x(H') \) to denote the operator \( H' \) involved. Finally, since \( 0 \leq \mu_x(\Delta) \leq \| \eta_x \|^2 \sup_{E \in \Delta} p_k(E)^2 \), we see that \( \mu_x \) is polynomially bounded.

After these preliminaries, we come to the statement of our dynamical quantum inequalities.

\(^7\)Since, for any \( \psi \in \mathcal{H} \), we have \( P_\Delta \psi \in D(p(H)) \), it follows that \( (P_\Delta \psi)(x) = \int dy P_\Delta(x, y) \psi(y) \) where \( P_\Delta(x, y) = (p_k(H)P_\Delta \eta_x)(y) \) is continuous in \( y \). This last quantity may easily be expressed as \( \langle p(H)P_\Delta \eta_x \mid p_k(H)P_\Delta \eta_y \rangle \), so in particular, \( P_\Delta(x, x) = \| p_k(H)P_\Delta \eta_x \|^2 = \mu_x(\Delta) \).
(III) Let \( g \) be any real-valued, compactly supported function on \( \mathbb{R} \) and set \( f = g^2 \). Then given real numbers \( a < b \), the inequalities
\[
 b \langle \rho_x(f) \rangle_\psi + \int \frac{du}{2\pi} Q_+(u) |\tilde{g}(u)|^2 \geq \langle h_x(f) \rangle_\psi \geq a \langle \rho_x(f) \rangle_\psi - \int \frac{du}{2\pi} Q_-(u) |\tilde{g}(u)|^2
\]
hold for all normalised \( \psi \in P_{[a,b]} \mathcal{H} \), where
\[
 Q_-(u) = \int_{[a,b]} d\mu_x(E) \{ hu + a - E \}_+ \\
 Q_+(u) = \int_{[a,b]} d\mu_x(E) \{ hu - b + E \}_+
\]
are nonnegative, monotone increasing and polynomially bounded in \( u \), and we have used the notation \( \{ \lambda \}_+ = \max\{0, \lambda\} \). (Similarly, we will write \( \{ \lambda \}_- = \min\{0, \lambda\} \).) Moreover, the first (resp., second) inequality in (4.10) also holds for all \( \psi \in P_{(-\infty,b]} \mathcal{H}_{k+1} \) (resp., \( P_{[a,\infty)} \mathcal{H}_{k+1} \)) provided the integration range in (4.11) is replaced by \( (-\infty, b] \) (resp., \( [a, \infty) \)).

(IV) Suppose \( \int_{\mathbb{R}} d\mu_x(E) (1 + |E|) < \infty \) and let \( g \) be as in (III). Then, for any fixed \( c \in \mathbb{R} \), the inequality
\[
 \langle h_x(f) \rangle_\psi \geq c \langle \rho_x(f) \rangle_\psi - \int \frac{du}{2\pi} S(H - c1; u) |\tilde{g}(u)|^2
\]
holds for all \( \psi \in \mathcal{H}_{k+1} \), where
\[
 S(H; u) = \int d\mu_x^{(H)}(E) \{ hu - E \}_+
\]
is nonnegative, monotone increasing and polynomially bounded in \( u \). (There is of course a dual statement, for the case \( \int_{\mathbb{R}} d\mu_x(E) (1 + |E|) < \infty \).)

Before proceeding to the proof of these statements, we illustrate them by drawing some consequences. The interpretation of (III) is that a state with energy between \( a \) and \( b \) has an averaged energy density between \( a \) and \( b \), suitably weighted by the averaged position probability density, modulo a certain latitude bounded by quantum inequalities. Replacing \( g \) by \( g_\lambda(t) = \lambda^{-1/2} g(t/\lambda) \), we may consider the two regimes \( \lambda \to 0^+ \), representing tightly peaked averages, and \( \lambda \to \infty \), which represents widely spread averages. In the former case, we have
\[
 \int \frac{du}{2\pi} Q_\lambda(u) |\tilde{g}_\lambda(u)|^2 \sim \frac{\mu_x([a,b])}{\lambda} \int_0^\infty \frac{du}{2\pi} u |\tilde{g}(u)|^2
\]
provided \( \mu_x([a,b]) > 0 \) (failing which the left-hand side vanishes identically). Thus the latitude afforded by the quantum inequality bound grows as the sampling becomes more tightly peaked. As \( \lambda \to \infty \), the QI latitude tends to zero and one may show that
\[
 b \geq \limsup_{\lambda \to \infty} \frac{\langle h_x(g_\lambda^2) \rangle_\psi}{\langle \rho_x(g_\lambda^2) \rangle_\psi} \geq \liminf_{\lambda \to \infty} \frac{\langle h_x(g_\lambda^2) \rangle_\psi}{\langle \rho_x(g_\lambda^2) \rangle_\psi} \geq a \tag{4.15}
\]
for all \( \psi \in P_{[a,b]} \mathcal{H} \), provided \( \langle \rho(t, x) \rangle_\psi \) is nonzero for some \( t \). This ergodic result shows that the spatial and temporal averages of energy densities obey related constraints.

As a second illustration, consider (IV) in the case where \( H \) has a discrete spectrum \( \{E_n\} \) with corresponding orthonormal eigenfunctions \( \{\phi_n\} \), and satisfying the integrability condition on \( \mu_x \) (for example, \( H \) might be semibounded). Then, in the case \( c = 0 \),

\[
\langle h_x(g^2) \rangle_\psi \geq - \int \frac{du}{2\pi} |\hat{g}(u)|^2 \sum_{E_n \leq u} |\phi_n(x)|^2 (hu - E_n) = - \sum_n \alpha_n |\phi_n(x)|^2
\]

(4.16)

where

\[
\alpha_n = \int_{E_n}^\infty du |\hat{g}(u)|^2 (hu - E_n).
\]

(4.17)

These formulae may be used to compare the relative ease of obtaining negative energy densities at different spatial locations. For example, the eigenfunctions \( \phi_n \) of the harmonic oscillator \( H = p^2/(2m) + \frac{1}{2}m\omega^2 x^2 \) on \( L^2(\mathbb{R}) \) obey the following bounds (cf. the Appendix to Sec. V.3 in [35]): For any \( j \in \mathbb{N}_0 \) there exists \( c_j > 0 \) and \( r_j \in \mathbb{N}_0 \) such that

\[
\sup_{x \in \mathbb{R}} |(1 + x^j)\phi_n(x)| \leq c_j (1 + n)^{r_j}
\]

(4.18)

for all \( n \in \mathbb{N}_0 \). Thus, for all normalised \( \psi \in \mathcal{S}(\mathbb{R}) \) (in fact, for all \( \psi \) in a considerably larger domain) we have

\[
\langle h_x(g^2) \rangle_\psi \geq - \frac{c_j}{1 + |x|^j} \sum_{n=0}^\infty \alpha_n (1 + n)^{r_j}.
\]

(4.19)

In this case, it is clear that—for a fixed sampling function \( g \)—the \( \alpha_n \) form a rapidly decaying sequence and so the sum converges for any \( j \). Thus we have shown that the state-independent bound on energy density is itself a rapidly decaying function of \( x \). It is therefore generally easier to maintain negative energy densities near the classical equilibrium point rather than far away.

Finally, consider (III) for the case \( H = -id/dx \) on \( \mathcal{H} = L^2(\mathbb{R}) \) and a particle of mass \( m \). In this instance, the spaces \( \mathcal{H}_k \) coincide with the Sobolev spaces \( W^{k,2}(\mathbb{R}) \) and Sobolev’s lemma permits us to take \( k > 1/2 \). Then the dynamical evolution amounts to spatial translation and the averaged Hamiltonian density is related to the spatially averaged probability flux by

\[
\langle h_x(f) \rangle_\psi = mj_\psi(\tilde{f}_x)
\]

(4.20)

where \( \tilde{f}_x(t) = f(x - t) \). Moreover, the measure \( \mu_x \) is easily seen to be given by \( \mu_x(\Delta) = |\Delta|/(2\pi \hbar) \), where \( |\cdot| \) denotes the usual Lebesgue measure. Then the second inequality in (III) may easily be checked to reproduce the flux inequality \((2.10)\) for all \( \psi \in P_{[0,\infty]} W^{k+1,2}(\mathbb{R}) \).

The remainder of this section is devoted to the proof of statements (III) and (IV). These
assertions are based upon two facts, which will be proved below. First, for any \( c \in \mathbb{R} \) and normalised \( \psi \in \mathcal{H}_{k+1} \), one may show that
\[
\langle h_x(f) \rangle_\psi - c \langle \rho_x(f) \rangle_\psi = \int \frac{d\epsilon}{2\pi\hbar} \left( \epsilon - c \right) \left| \langle \psi \mid p_k(H) \hat{g}(\hbar^{-1}[\epsilon - H]) \eta_x \rangle \right|^2. \tag{4.21}
\]
Second, if \( \Delta \) is a Borel set then
\[
\left| \langle \psi \mid p_k(H) \hat{g}(\hbar^{-1}[\epsilon - H]) \eta_x \rangle \right|^2 \leq \int_{\Delta} d\mu_x(E) \left| \hat{g}(\epsilon - E) / h \right|^2. \tag{4.22}
\]
for all normalised \( \psi \in P_{\Delta \mathcal{H}} \). Putting these together, we obtain
\[
\langle h_x(f) \rangle_\psi - c \langle \rho_x(f) \rangle_\psi \geq \int \frac{d\epsilon}{2\pi\hbar} \left( \epsilon - c \right) \int_{\Delta} d\mu_x(E) \left| \hat{g}(\epsilon - E) / h \right|^2
\]
\[
= \int \frac{d\mu_x(E)}{2\pi} \left| \hat{g}(u) \right|^2 \int_{\Delta} d\mu_x(E) \left\{ hu + E - c \right\}_-, \tag{4.23}
\]
for all normalised \( \psi \in P_{\Delta \mathcal{H}} \), where we have made the change of variables \( u \to -u \) and exploited the fact that \( \left| \hat{g}(u) \right|^2 \) is even (because \( g \) is real-valued). The interchange of variables employed in the first step is justified provided the inner integral in the last line of (4.23) is polynomially bounded in \( u \).

To obtain the second inequality in (III), we set \( c = a \) and \( \Delta = [a, b] \) and observe that the inner integral in Eq. (4.23) reduces to \( Q_-(u) \) and is polynomially bounded because \( \mu_x \) is. The inequality clearly remains true for \( \psi \in P_{[a, \infty) \mathcal{H}_{k+1}} \) with \( \Delta = [a, \infty) \). To obtain (IV), we set \( \Delta = \mathbb{R} \) and observe that the integrability condition \( \int_{\mathbb{R}} d\mu_x(E)(1 + |E|) < \infty \) and polynomial boundedness of \( \mu_x \) guarantee that \( S(H - c\mathbb{I}, u) \) exists and is polynomially bounded. Inequality (4.12) follows from the above on observing that \( \int d\mu_x(H)(E) F(E - c) = \int d\mu_x^{(H - c\mathbb{I})(E)} F(E) \).

To obtain the first inequality in (III) and the dual statement to (IV), one argues in an analogous fashion from the calculation
\[
\langle h_x(f) \rangle_\psi - c \langle \rho_x(f) \rangle_\psi \leq \int \frac{d\epsilon}{2\pi\hbar} \left( \epsilon - c \right) \int_{\Delta} d\mu_x(E) \left| \hat{g}(\epsilon - E) / h \right|^2
\]
\[
= \int \frac{d\mu_x(E)}{2\pi} \left| \hat{g}(u) \right|^2 \int_{\Delta} d\mu_x(E) \left\{ hu + E - c \right\}_+. \tag{4.24}
\]
which holds for all normalised \( \psi \in P_{\Delta \mathcal{H}} \).

It remains to prove the two facts presented as Eqs. (4.21) and (4.22) above. First, observe that for any normalised \( \psi \in \mathcal{H}_k \), \( \langle \rho_x(f) \rangle_\psi \) may be expressed as
\[
\langle \rho_x(f) \rangle_\psi = \int dt f(t) \int d\langle \psi \mid P_E \eta_x \rangle \int d\langle \eta_x \mid P_E \psi \rangle e^{i(E - E')t / \hbar} \rho_k(E) p_k(E') \tag{4.25}
\]
by the functional calculus. Performing the \( t \) integral first (which is legitimate since \( f \) is smooth and compactly supported) we obtain
\[
\langle \rho_x(f) \rangle_\psi = \int d\langle \psi \mid P_E \eta_x \rangle \int d\langle \eta_x \mid P_E \psi \rangle \hat{f}([E' - E] / h) \rho_k(E) p_k(E'). \tag{4.26}
\]

20
Since \( f = g^2 \), the convolution theorem may be used to write

\[
\hat{f}([E' - E]/\hbar) = \int \frac{d\epsilon}{2\pi\hbar} \overline{\hat{g}([E' - \epsilon]/\hbar)\hat{g}([E - \epsilon]/\hbar)}
\]  

(4.27)

using the fact that \( \overline{\hat{g}(\lambda)} = \hat{g}(-\lambda) \) since \( g \) is real-valued. Substituting in (4.26), and again rearranging the order of integration, we obtain

\[
\langle \rho_x(f) \rangle_\psi = \int \frac{d\epsilon}{2\pi\hbar} \int d\langle \psi \mid P_E\eta_x \rangle \int d\langle \eta_x \mid P_{E'}\psi \rangle \hat{g}([E' - \epsilon]/\hbar) \overline{\hat{g}([E - \epsilon]/\hbar)p_k(E)p_k(E')} \\
= \int \frac{d\epsilon}{2\pi\hbar} \left| \int d\langle \psi \mid P_E\eta_x \rangle p_k(E) \overline{\hat{g}([E - \epsilon]/\hbar)} \right|^2 \\
= \int \frac{d\epsilon}{2\pi\hbar} \left| \langle \psi \mid p_k(H)\hat{g}(\hbar^{-1}[\epsilon\mathbb{1} - H])\eta_x \rangle \right|^2
\]  

(4.28)

To treat \( \langle h_x(f) \rangle_\psi \) for normalised \( \psi \in \mathcal{H}_{k+1} \), we write

\[
\langle h_x(f) \rangle_\psi = \frac{1}{2} \int dt \, f(t) \int d\langle \psi \mid P_E\eta_x \rangle \int d\langle \eta_x \mid P_{E'}\psi \rangle e^{i(E - E')t/\hbar}(E + E')p_k(E)p_k(E'),
\]  

(4.29)

by functional calculus and use the identity

\[
\frac{(E + E')}{2} \hat{f}([E' - E]/\hbar) = \int \frac{d\epsilon}{2\pi\hbar} \epsilon \overline{\hat{g}([E' - \epsilon]/\hbar)\hat{g}([E - \epsilon]/\hbar)}
\]  

(4.30)

in place of the convolution theorem. (See \[19\] and \[15\] for proofs of this identity.) By a derivation analogous to that used for \( \langle \rho_x(f) \rangle_\psi \) we then obtain

\[
\langle h_x(f) \rangle_\psi = \int \frac{d\epsilon}{2\pi\hbar} \epsilon \left| \langle \psi \mid p_k(H)\hat{g}(\hbar^{-1}[\epsilon\mathbb{1} - H])\eta_x \rangle \right|^2
\]  

(4.31)

and Eq. (4.21) follows from this equation and (4.28).

The second assertion, Eq. (4.22), is proved by noting that

\[
\left| \langle \psi \mid p_k(H)\hat{g}(\hbar^{-1}[\epsilon\mathbb{1} - H])\eta_x \rangle \right|^2 \leq \left\| p_k(H)\hat{g}(\hbar^{-1}[\epsilon\mathbb{1} - H])\eta_x \right\|^2
\]  

(4.32)

using \( \psi = P_\Delta \psi \) and the Cauchy–Schwarz inequality (with \( \|\psi\| = 1 \)). The right-hand side may be written

\[
\int_\Delta d\langle \eta_x \mid P_E\eta_x \rangle p_k(E)^2 \left| \hat{g}([\epsilon - E]/\hbar) \right|^2 = \int_\Delta d\mu_x(E) \left| \hat{g}([\epsilon - E]/\hbar) \right|^2
\]  

(4.33)

which completes the derivation of Eq. (4.22).

5 Numerical Details

In this section we provide more details on the numerical methods employed in Sect. 2 and discuss rigorous error estimates on the numerical errors. The basic numerical method is
easily explained (see, e.g., Sec 4.1 of [4] or Chapter 4 of [10]). Suppose \( T \) is an integral operator on \( L^2(\mathbb{R}^+, dk) \) with kernel \( G \), i.e.,

\[
(T\psi)(k) = \int_0^\infty dk' G(k, k') \hat{\psi}(k').
\]

To handle this numerically, we first truncate the kernel to \([0, K] \times [0, K]\) for some \( K > 0 \), which amounts to studying a compression \( T_K \) of \( T \). Provided that the required properties of \( T \) are, for sufficiently large \( K \), well-approximated by the corresponding properties of \( T_K \) restricted to \( L^2(0, K) \), we proceed to approximate this restricted operator by a matrix.

To do this, we suppose that \((\xi_j)_{j=0}^N\) and \((w_j)_{j=0}^N\) are the nodes and weights for a suitable quadrature method on \([0, K]\), and define the \((N + 1)\)-square matrix \( A = (A_{jk})_{j,k=0}^N \) with \((j, k)\) entry \( A_{jk} = w_j^{1/2} w_k^{1/2} G_{\lambda,k}(\xi_j, \xi_k) \). The relevant computations are performed on \( A \) and, if \( N \) and \( K \) are sufficiently large, this will provide a numerical approximation to the required quantity.

This technique was applied to the Bracken–Melloy kernel as described in Sect. 2.2. In that case, we were unable to derive useful error estimates. However, the operator norm calculations of Sect. 2.3 are more controlled, as we now describe. The problem is to estimate the squared operator norms of the family of integral operators \( T_\lambda \) \((\lambda > 0)\) defined in the above fashion\(^8\) with kernel

\[
G_{\lambda,k}(k, k') = \frac{1}{2\pi} \sqrt{k} \hat{g}_\lambda(-k - k').
\]

Now the compressions \( T_{K,\lambda} \) converge to \( T_\lambda \) in the Hilbert–Schmidt norm, and therefore in operator norm, as \( K \to \infty \). That the matrix approximations have operator norms converging to \( \|T_{K,\lambda}\| \) as \( N \to \infty \) is a consequence of the convergence of the quadrature formula to the integral for continuous functions. Thus our technique may be validly applied to this problem and it remains to control the errors inherent in the scheme for finite \( N \) and \( K \). In general we have analytical control of the truncation errors (parametrised by \( K \)) but not the discretisation errors; we are, however, able to observe apparent convergence to machine precision in most cases. As a first step in our analysis of the truncation errors, we eliminate the parameter \( \lambda \) from our considerations: \( G_{\lambda} \) and the dilation of \( G_1 \) by a factor of \( \lambda \) differ only by a constant factor of \( \lambda \), so if truncation of \( G_1 \) at \( K \) has a relative error of \( \varepsilon \) (in either Hilbert–Schmidt or operator norm) then truncation of \( G_{\lambda} \) at \( \lambda K \) also has relative error \( \varepsilon \), and the associated quadrature matrices are identical apart from a factor of \( \lambda \). From now on, we will use the value \( \lambda = 1 \) only, and write \( T_K \) for \( T_{K,1} \), etc.

In order to estimate truncation errors, the following observations are useful. We wish to integrate \( |G|^2 \) over the region \([0, \infty) \times [0, \infty) \setminus [0, K] \times [0, K]\). By symmetry we can integrate \((|G(k, k')|^2 + |G(k', k)|^2)/2\) over the same region to obtain the same result. This has the advantage that

\[
\frac{|G(k, k')|^2 + |G(k', k)|^2}{8\pi^2} = \frac{(k + k')|\hat{g}(-k - k')|^2}{8\pi^2}
\]

which depends only on \( k + k' \). We can exploit this by using the following decomposition of the quadrant \([0, \infty) \times [0, \infty)\)

\(^8\)In Sect. 2.3, the operators were defined on \( L^2(\mathbb{R}^+, dk/(2\pi)) \). Here, we absorb the factor of \((2\pi)^{-1}\) into the kernel, which leaves the spectral data and operator norms unchanged.
We wish to evaluate the integral over $R_1 \cup R_2 \cup R_3$, and by symmetry the integrals over $R_1$ and $R_2$ are equal. Changing into a $(k + k', k - k')$ coordinate system we see that the required integral is

$$\frac{1}{4\pi^2} \int_K^{2K} u(u - K)|\hat{g}(-u)|^2 du + \frac{1}{8\pi^2} \int_{2K}^{\infty} u^2|\hat{g}(-u)|^2 du.$$  \hspace{1cm} (5.4)

We now consider the four sampling functions used in Sect. 2.3. Starting with the Gaussian kernel

$$\hat{g}(k) = \sqrt{2\pi}^{1/4} e^{-k^2/2},$$  \hspace{1cm} (5.5)

the Hilbert–Schmidt norm of $T$ can be found by substituting $K = 0$ in (5.4) and evaluating the integral to give

$$\|T\|_{\text{H.S.}} = \frac{1}{4\sqrt{\pi}}$$  \hspace{1cm} (5.6)

which is of course an upper bound for the operator norm.

For more precise results, we turn to the quadrature method described above. For this kernel, the integrals in (5.4) can be evaluated explicitly to give a relative error in the Hilbert-Schmidt norm of

$$\frac{\|T - T_K\|_{\text{H.S.}}}{\|T\|_{\text{H.S.}}} = (1 + \text{erf}(2K) - 2 \text{erf}(K))^{1/2}.$$  \hspace{1cm} (5.7)

It can be numerically verified that the relative error falls below $\varepsilon = 0.5 \times 10^{-10}$ (for ten-digit precision) at approximately $K = 6.756$ (this calculation requires about 25-digit precision).

The computations were performed in Maple 8 using $c$-panel repeated Clenshaw-Curtis quadrature (see Section 2.4.4 of [10]) on the interval $[0, 6.9]$ and Maple’s NAG-based `SingularValues` routine. Using 33, 65 or 129 samples with $c = 1.2$ gives in each case the same results for the first largest two singular values: $\sigma_1 = 0.1399331442$, $\sigma_2 = 0.0175697912$ to 10 figures. Notice that the second singular value is very much smaller than the first, which means that the matrices, and hence $T$, can be well approximated by operators of rank 1. This is consistent with the operator norm, computed here to be .1399331442, being close to the Hilbert-Schmidt norm, $1/(4\sqrt{\pi}) = .1410473959\ldots$. This similarity finally justifies our use of truncation constants based on the relative error in the
Hilbert-Schmidt norm: the calculated value of the operator norm is certainly no larger than the true value, since it is the norm of a compression of $T$, so we have

$$\frac{\|T - T_K\|}{\|T\|} \leq \frac{\|T - T_K\|_{\text{H.S.}}}{\|T\|_{\text{H.S.}}} \|T\|_{\text{H.S.}}$$

$$\leq 0.4873572016 \times 10^{-10} \times 0.1410473959 \times 0.1399331442 = 0.4912379017 \times 10^{-10} \quad (5.8)$$

which is still less than the target figure of $0.5 \times 10^{-10}$.

The next kernel of interest is the squared Lorentzian; however, in this case $T$ is a rank-1 operator so the Hilbert–Schmidt and operator norms coincide and there is no need for numerical investigation. This leaves the two compactly supported kernels. In the truncated cosine case, the same techniques as above lead to an error estimate of the order of 2% relative error in the Hilbert–Schmidt norm for $K = 1100$. As this is a rather weak estimate, we suppress the details; the numerical estimate of the squared operator norm (for $K = 1100$, $N = 1024$) is given in Sect. 2.3.

Our last example is the smoothed truncated cosine, defined by

$$\hat{g}(k) = \frac{2\sqrt{3}\pi^2}{3} \frac{\sin(k)}{(\pi^2 - k^2)^{3/2}}. \quad (5.9)$$

The relatively slow decay of this function makes the precision obtained in the Gaussian example impractical, but we can obtain results to at least four significant figures. In fact the numerical results appear to be much more precise than would be suggested by this error estimate.

Maple is able explicitly to evaluate the integrals in (5.4) to give a rather complicated formula involving the $\text{Si}$ and $\text{Ci}$ special functions, and from this to give the asymptotic formula

$$\frac{5\pi}{16K^3} + o\left(\frac{1}{K^4}\right) \quad (5.10)$$

for the relative error in the Hilbert-Schmidt norm. Using only the leading term, we can predict that truncation at about $K = 732.3$ should give a Hilbert-Schmidt norm relative error less than $0.5 \times 10^{-4}$; numerical investigation of the exact formula near this point confirms this value. Proceeding in the same way as for the Gaussian kernel but this time using the faster numerical engine in Matlab 6 to calculate the singular values, we obtain the following results ($N + 1$ samples, $c$ panels):

| $N$ | $c$ | $\sigma_1$ | $\sigma_2$ |
|-----|-----|------------|------------|
| 256 | 1   | 0.3536210415 | 0.0733902393 |
| 256 | 2   | 0.3536211355 | 0.0733900951 |
| 512 | 1   | 0.3536210388 | 0.0733902259 |
| 512 | 2   | 0.3536210388 | 0.0733902259 |
| 1024| 1   | 0.3536210388 | 0.0733902259 |
| 1024| 2   | 0.3536210388 | 0.0733902259 |

Once again, the fact that the second singular value is considerably smaller than the first can be used after the fact to justify the use of relative errors in the Hilbert-Schmidt norm (rather than in the operator norm) in choosing the truncation constant.
Although the error analysis only allows us to be confident of the first four figures, it seems likely that this figure for the operator norm is considerably more accurate than that. Doubling the truncation constant and using 2049 points, again with 1 and 2 panels, gives exactly the same results to ten figures as the two 1025-point methods above.

The last set of calculations reported in Sect. 2.3 concern the unbounded operator $J$ of Eq. (2.20). Here we have not succeeded in obtaining usable estimates of the errors introduced by truncation to $[0,K]$. However, it is nonetheless true that $\inf \sigma(J_K) \to \inf \sigma(J)$ as a consequence of the following arguments.

**Proposition** Suppose $k$ is an absolutely bounded kernel on $L^2(0,\infty)$, and let $w$ be a measurable function on $(0,\infty)$ (with respect to Lebesgue measure). Let

$$D = \{ f \in L^2(0,\infty) : w f \in L^2(0,\infty) \}.$$  

Suppose $(w(x)+w(y))k(x,y)$ is a Hermitian function of $x$ and $y$, and define an operator with domain $D$ by

$$(Tf)(x) = \int_0^\infty (w(x)+w(y))k(x,y)f(y)dy$$

and assume that $T$ is bounded below. For $K > 0$ define the truncated operator

$$(T_Kf)(x) = \int_0^K (w(x)+w(y))k(x,y)f(y)dy.$$  

Then

$$\lim_{K \to \infty} \inf \sigma(T_K) = \inf \sigma(T).$$

**Proof:** $T_K$ is a compression of $T$ so $\inf \sigma(T_K) \geq \inf \sigma(T)$ for all $K$. For any $\varepsilon > 0$ we can choose $f \in D$ with $\|f\| = 1$ and such that $\langle f \mid Tf \rangle < \inf \sigma(T) + \varepsilon/2$. Now

$$\langle f \mid Tf \rangle = \int_0^\infty \int_0^\infty (w(x)+w(y))k(x,y)f(y)dy f(x)dx$$

and the integrand here is in $L^2((0,\infty) \times (0,\infty))$ by the lemma. It now follows from Lebesgue’s dominated convergence theorem and Fubini’s Theorem that, provided the above repeated integral can be interpreted as an integral on the measure space $(0,\infty) \times (0,\infty)$,

$$\langle f \mid Tf \rangle = \lim_{K \to \infty} \int_0^K \int_0^K (w(x)+w(y))k(x,y)f(y)dy f(x)dx.$$  

If we let $f_K(x) = f(x)\chi_{(0,K)}(x)$ then this tells us that $\langle f_K \mid T_K f_K \rangle \to \langle f \mid Tf \rangle$; we also have $\|f_K\| \to \|f\| = 1$ as $K \to \infty$, so $\langle f_K \mid T_K f_K \rangle/\|f_K\|^2 \to \langle f \mid Tf \rangle$ as $K \to \infty$. In particular, for sufficiently large $K$ we have

$$\frac{\langle f_K \mid T_K f_K \rangle}{\|f_K\|^2} < \frac{\varepsilon}{2} < \inf \sigma(T) + \varepsilon$$

which implies that $\inf \sigma(T_K) < \inf \sigma(T) + \varepsilon$. In combination with the earlier inequality $\inf \sigma(T_K) \geq \inf \sigma(T)$, this establishes the result.
It remains to justify the treatment of the repeated integral as an integral on a product measure space.

**Lemma** In the notation of the above theorem, for any \( f, g \in D \), the repeated integral in the bilinear form

\[
\int_0^\infty \left( \int_0^\infty (w(x) + w(y))k(x, y)f(x)g(y)dy \right) dx
\]

is absolutely convergent, and so can be interpreted as the integral of a function in \( L^2((0, \infty) \times (0, \infty)) \).

**Proof:** We calculate

\[
\int_0^\infty \left( \int_0^\infty |(w(x) + w(y))k(x, y)f(x)g(y)|dy \right) dx \\
\leq \int_0^\infty \left( \int_0^\infty (|w(x)| + |w(y)|)|k(x, y)||f(x)||g(y)|dy \right) dx \\
= \int_0^\infty \left( |f(x)w(x)| \int_0^\infty |k(x, y)||g(y)|dy \right) dx + \\
\int_0^\infty \left( |f(x)||k(x, y)||w(y)g(y)|dy \right) dx. \tag{5.19}
\]

In the first term, the inner integral defines an \( L^2 \) function of \( x \) since \( k \) is an absolutely bounded kernel, and \( f(x)w(x) \) is an \( L^2 \) function of \( x \) since \( f \in D \). The first term is therefore finite by the Cauchy-Schwarz inequality. The second term is finite by similar reasoning: \( w(y)g(y) \) is an \( L^2 \) function of \( y \) since \( g \in D \), so the inner integral define an \( L^2 \) function of \( x \), and \( f \) is \( L^2 \) by hypothesis. The final conclusion now follows from Tonelli’s Theorem.

## 6 Conclusion

The main focus of this paper has been to draw attention to links between the failure of pointwise energy conditions in quantum field theory and a range of similar situations in quantum mechanics. In addition we have seen that there are links at the technical level between the QIs developed in quantum field theory and those obtained here in the quantum mechanical setting. In addition, we have made contact with the ideas and methods of Weyl–Wigner quantisation and sharp Gårding inequalities. In conclusion, we briefly summarise the new results we have obtained along the way.

First, we have seen that the backflow phenomenon is limited in space (as well as in time [7]) as shown by our flux QI (2.10). In particular, the magnitude of the negative flux times the square of its spatial extent is bounded above for all right-moving states in \( \mathcal{R} \). We have also provided an improved numerical estimate of Bracken and Melloy’s backflow constant, and also given numerical evidence to support the conjecture that our flux QI is generally within an order of magnitude of the optimal bound (i.e., the infimum of the spectrum of \( J \), given by Eq. 2.26).
Second, we have shown that similar phenomena occur for densities of observables ob-
tained via Weyl quantisation. This is a consequence of the indefinite sign of the Wigner
function, and therefore an expression of the uncertainty principle. Moreover, for observ-
ables which are second order (or less) in momentum, we have seen that sharp Gårding
inequalities entail the existence of kinematic quantum inequalities. We have also obtained
explicit bounds in the case of Schrödinger operators with smooth potentials.

Finally, for general quantum mechanical systems describing dynamics on a topological
measure space, we have shown that the time-averaged energy density obeys dynamical
quantum inequalities (evolution being generated by the spatial integral of the energy
density). For the 1-dimensional harmonic oscillator, we saw that the QI bound (for a
given sampling function) is a Schwartz-class function: it becomes rapidly much harder
to create sustained negative energy densities away from the classical equilibrium point.
Moreover, we have seen that a bound on the spectral behaviour of the Hamiltonian on
the negative spectral axis, expressed by the integrability condition on $\mu_\alpha$ in (IV), already
leads to dynamical QIs. This integrability condition can be viewed as a condition on the
global dynamical stability of a quantum system, much in the sense of quantum systems
in thermal equilibrium, where the spectral weight of the generator of the time-evolution
(the Liouvillian) is exponentially suppressed on the negative half-axis (cf. Prop. 5.3.14 in
[8]). This indicates again the link between (thermo)dynamical stability and dynamical
QIs which was established in [20] and which originally motivated the introduction of QIs in
[22].

All these findings corroborate the intimate connection between QIs and the fundamen-
tal principles of quantum mechanics: the uncertainty principle and dynamical stability.

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