Exact energy–time uncertainty relation for arrival time by absorption

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Abstract

We prove an uncertainty relation for energy and arrival time, where the arrival of a particle at a detector is modeled by an absorbing term added to the Hamiltonian. In this well-known scheme the probability for the particle’s arrival at the counter is identified with the loss of normalization for an initial wave packet. Under the sole assumption that the absorbing term vanishes on the initial wavefunction, we show that $\Delta T \Delta E \geq \sqrt{p \hbar}/2$ and $\langle T \rangle \Delta E \geq 1.37 \sqrt{p \hbar}$, where $\langle T \rangle$ denotes the mean arrival time and $p$ is the probability for the particle to be eventually absorbed. Nearly minimal uncertainty can be achieved in a two-level system, and we propose a trapped ion experiment to realize this situation.

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1. Introduction

From Heisenberg’s seminal 1927 paper [1], uncertainty relations have been recognized as a fundamental feature of quantum mechanics. Heisenberg gives a semi-classical heuristic discussion and his ‘uncertainties’ are conceptually different in different parts of his paper. Accordingly, they are not given a precise quantitative meaning in the mathematical language of quantum theory. On the other hand, modern textbooks all agree on ‘the’ uncertainty relation, namely a version stated and proved by Kennard [2] in the same year Heisenberg’s paper appeared. Kennard achieved an important clarification both conceptually, by defining the uncertainties as the standard deviation of operationally well-defined probability distributions, and also quantitatively, so it becomes possible to say that some experiment realizes an uncertainty product within 3% of the absolute minimum. This clarification was so successful that other aspects of Heisenberg’s paper, like his discussion of the precision of a position measurement by microscope versus the momentum disturbance by the measurement, fell into
disrepute. Nevertheless, these ideas are not only heuristically meaningful, but can be made operationally precise and proved as theorems in the quantum formalism [3, 4]. Another group of sharp results looks at the position and momentum distributions like Kennard, but defines the ‘spread’ in a different way. Particularly interesting is a non-parametric version in terms of entropies [5–7], which has applications in cryptography [8]. Since many experiments are nowadays approaching quantum limits, it is perhaps becoming more important to think of uncertainty relations not as a single fact, but as a circle of ideas in which traditional heuristic interpretations coexist with an increasing family of exact results.

The ambiguities in the literature multiply when we go from position–momentum uncertainty to energy–time uncertainty. In most cases, energy–time uncertainty relations are invoked in a handwaving fashion only. There are very few conceptually clear and quantitatively meaningful formulations (see [9] for a review). In this article, we use an interpretation which is related as closely as possible to Kennard’s interpretation of $\Delta P$ and $\Delta Q$: We take both quantities as the standard deviations of some probability distributions: $\Delta E$ is the standard deviation of the energy observable (the Hamiltonian) of the system and $\Delta T$ is the standard deviation of arrival time. This is to be thought of as the distribution of times at which a detector clicks relative to some trigger signal of the preparation. Such measurements are commonplace in the lab, but the observables needed for their theoretical description are not so widely known. Workarounds using instead the time-dependent position probability density (resp. the probability current) fail for reasons of normalization (resp. positivity). One way for a correct modeling of such an arrival time detection process is by so-called covariant observables [10–12]. These are positive operator valued measures on the time line with the property that preparing systems some time later, i.e. by acting on the initial state with the unitary evolution operator, one always obtains an accordingly shifted time distribution. For any such observable the Kennard-like uncertainty relation holds [13]. However, this notion of arrival times is rather inflexible and makes no sense for finite dimensional systems. These drawbacks can be cured in a more realistic theory of arrival times [14–16], in which the counter is modeled by an absorbing term in the Hamiltonian.

The purpose of this paper is to provide a sharp quantitative formulation of uncertainty for energy and absorptive arrival time. The possibility of such an uncertainty relation is somewhat surprising (and totally missed in the literature, including [15]), since the dynamics including the counters, which is used to define $\Delta T$, is not generated by the Hamiltonian used to define $\Delta E$, so there would appear to be no universal trade-off inequality. Nevertheless, we will prove such a relation under only a mild and natural assumption on the initial state. An immediate advantage of the absorptive arrival time approach is that it also applies to certain finite dimensional models used in quantum optics.

The precision of quantum optical experiments and even of some experiments with massive particles has reached the scale where energy–time uncertainty becomes visible. To illustrate this point, we include the description of a concrete minimal uncertainty experiment with trapped ions.

Our paper is organized as follows. After a brief introduction to absorptive arrival times, we will state the relation and the conditions for near-equality. The main ideas of the proof are sketched in the following section, with a full proof given in the appendix. We then show that (very nearly) minimum uncertainty can be realized in a standard quantum optical setting.

2. Arrival times

Consider a quantum system with Hilbert space $\mathcal{H}$ and time-independent Hamiltonian $H$. Starting from some initial state $\psi \in \mathcal{H}$, we would like to determine the probability
distribution of arrival times at some counter. There are different approaches to this problem, varying in the degree of detail with which the counter is described.

The coarsest, and simplest, description focuses just on transformation behavior: starting from the time-evolved state \( \psi_t = \exp(-iHt/\hbar)\psi \) we should get the same arrival time distribution, but shifted by \( t \). Covariant arrival observables with this property have been studied extensively [10–12, 17], and satisfy a general energy–time uncertainty relation [13]. However, transformation behavior alone is not sufficient to single out a convincing model for a given experimental counter array. Moreover, this approach requires the Hamiltonian to have a purely continuous spectrum and is hence limited to infinite dimensional Hilbert spaces.

At the other extreme we can make a detailed detector model, e.g., by interaction with an ionizable atom [18]. The drawback of this scheme is that, although undoubtedly physically correct, the interacting system is very hard to treat, and a disproportionate amount of the analysis of a given experiment would go just into the detection process.

The absorptive arrival times approach adopted in this paper is a good compromise between these extremes: it was first worked out in detail in [14] and describes the detector by a non-Hermitian term \(-iD\) added to the Hamiltonian \( H \), which is thus replaced by \( K = H - iD \). Thereby the unitary time evolution operator \( U_t = \exp(-iHt/\hbar) \) is modified to a semigroup of contractions, i.e., operators \( \mathcal{B}_t = \exp(-iKt/\hbar) \) \((t \geq 0)\) such that \( \|\mathcal{B}_t\| \leq 1 \). We now interpret the loss of normalization, i.e. \( 1 - \|\mathcal{B}_t\psi\|^2 \), of a quantum state \( \psi \) as the probability that the particle did arrive before time \( t \). More generally, for any time interval \([t, s] \) with \( 0 \leq t \leq s \) the probability of arrival in that interval is given by the expectation of the operator

\[ F([t, s]) = \mathcal{B}_t^* \mathcal{B}_s - \mathcal{B}_t^* \mathcal{B}_s. \]

Thus, given a quantum state \( \psi \), we get a probability density \( \mathbb{P}(t) \) on the positive time axis by

\[ \mathbb{P}(t) = -\frac{1}{p} \frac{d}{dt} \langle \mathcal{B}_t \psi | \mathcal{B}_t \psi \rangle, \]

\[ p = 1 - \lim_{t \to \infty} \|\mathcal{B}_t\psi\|^2 = \langle \psi | (1-R) \psi \rangle. \]

Here the limit \( R = \lim_{t \to \infty} \mathcal{B}_t^* \mathcal{B}_t \) exists because it is over a decreasing family of positive operators, and \( p \) is the total absorption probability. For real detectors not every absorption actually leads to a detected click. Suppose the probability for this process is \( q \). Then we would observe a click in \([t, t + dt]\) with probability \( q \mathbb{P}(t) \, dt \). Hence \( \mathbb{P}(t) \) can be determined from the experimental data by normalizing the observed click distribution, independently of \( q \) or \( p \). The important distinction between these two probabilities is that the process leading from absorption to detection is independent of the particle dynamics and introduces no change in the further quantum evolution of the particle. Therefore, \( q \) cannot enter the uncertainty relation, but as we will see, \( p \) does.

We denote by \( \langle T \rangle \) and \( \langle T^2 \rangle \) the first and second moments of the probability distribution \( \mathbb{P}(t) \) after equation (2), and set \( \langle \Delta T \rangle^2 = \langle T^2 \rangle - \langle T \rangle^2 \). Defining \( \langle \Delta E \rangle^2 = \langle \psi | H^2 \psi \rangle - \langle \psi | H \psi \rangle^2 \), we can hence look for a universal lower bound on the product \( \Delta T \cdot \Delta E \).

Without further conditions such a lower bound cannot hold. Indeed, \( \Delta T \) can be computed knowing \( K \) and \( \psi \), whereas \( \Delta E \) depends on \( H \) and \( \psi \). For example, if we now set \( K = H - i\omega I \), we get \( p = 1 \) and \( \mathbb{P}(t) = 2\pi e^{-2\pi t} \) independently of \( \psi \). Clearly, this cannot imply any constraint on the energy distribution. Similarly, if the initial state is a joint eigenvector of \( H \) and \( K \), then \( \Delta E = 0 \) and \( \Delta T \) has a finite value belonging to an exponential distribution.

3. Uncertainty relation

From the last paragraph it seems that it makes no sense to look for a general time–energy uncertainty relation in this setting. However, as we will now show, a simple and physically
natural condition suffices to derive one. Loosely speaking, the condition is that the initial wavefunction has no overlap with the detector. More formally, if $D$ describes the detector as explained above, we want $D\psi = 0$, or $H\psi = K\psi$. Since these operators are usually unbounded, we also have to specify the domains. Writing $\text{dom} X$ for the domain of the operator $X$, we require that

$$\psi \in \text{dom} K \cap \text{dom} H \quad \text{and} \quad H\psi = K\psi.$$  \hfill (4)

The main result of our paper is that under this condition

$$\Delta T \cdot \Delta E > \frac{\hbar}{2} \sqrt{p}.$$  \hfill (5)

The dependence on $p$ expresses the fact that for a small detection operator $D$ only a few particles are ever detected ($p \approx 0$), so observing arrival times cannot imply a strong constraint on $\Delta E$. The power $\sqrt{p}$ is explained in the sketch of proof below. In the limiting case $D \to 0$, implying $p \to 0$, no particle arrives at all, and the arrival time distribution equation (2), including $\Delta T$ and $\langle T \rangle$ becomes ill defined. However, in this case the bound on the right-hand side also becomes trivial.

The arrival time distribution $P(t)$ is always supported by the positive time axis $\mathbb{R}_+$. Therefore, the mean arrival time $\langle T \rangle$ is always positive, and can take the place of $\Delta T$ in the uncertainty relation. Often $\langle T \rangle$ is of more immediate relevance than $\Delta T$. Consider, for example, the decay of a metastable state. The initial wavefunction is trapped inside a potential barrier, through which it will eventually tunnel. A detector is placed at a distance from the potential (so our initial condition $K\psi = H\psi$ is satisfied). Then $\langle T \rangle$ is directly an expression of the lifetime of the metastable state. Under the same conditions as for equation (5) we prove that

$$\langle T \rangle \cdot \Delta E \geq C \hbar \sqrt{p}$$  \hfill (6)

where $C = 2(-Z_1/3)^{3/2} \approx 1.376$ is a numerical constant involving the first negative zero $Z_1$ of the Airy function.

Cases of (nearly) minimal uncertainty are in both cases connected to specific probability distributions $P_{\text{min}}(t)$. Let $(1 + \varepsilon)$ denote the ratio of the left-hand side to the right-hand side in equation (5) or equation (6). Then, for a suitable scaling factor $\lambda$ and shift $\tau$,)

$$\int \text{d}t \left| P(t) - \lambda P_{\text{min}}(\lambda(t - \tau)) \right| \leq \gamma \sqrt{\varepsilon}$$  \hfill (7)

For equation (5), $P_{\text{min}}(t)$ is Gaussian, and $\gamma = \sqrt{2}$, as for the standard position–momentum uncertainty relation. For equation (6), $P_{\text{min}}(t)$ is the square of the Airy function, and $\gamma = 1.888$.

We remark that no such conclusion can be drawn for the energy distribution. In fact, although equation (5) is nearly sharp for the two-level system discussed below, the energy distribution is concentrated on two points, and is hence very different from a Gaussian. Another consequence is that equality (i.e. $\varepsilon = 0$) is impossible in equation (5), because every Gaussian has a tail extending to the negative half-axis. Equality is possible for equation (6), however.

4. Sketch of proof

The basic idea of the proof is a so-called dilation construction, by which the system is transformed in such a way that energy and time become conjugate self-adjoint operators, and theorems about position–momentum pairs can be used. The full argument allowing also unbounded $H$ and $K$ is given in the appendix. Here we give a rough version in theoretical physics (rather than mathematical) style. For simplicity we focus on the $\Delta E \Delta T$ relation.
equation (5), and assume that $K = H - iD$ for a bounded positive operator $D$. For the
dependence on the total absorption probability $p$ we only give an argument showing why the
square root is the expected power. For the main part of the proof we then just assume that
$p = 1$ for all initial states. This is true, e.g., in typical finite dimensional systems.

To understand the $\sqrt{p}$ factor in equations (5) and (6), consider some $\mathcal{H}, H, K, \psi$ as
above, with full absorption $p = 1$. Compare it with the following modification, which just
adds a part of the Hilbert space that is ‘not seen’ by the detector. Formally, the Hilbert
space $\mathcal{H}$ is enlarged by an additional orthogonal summand, on which $K$ vanishes, and which
contains an eigenvector $\phi_0$ of $H$ with $(\phi_0|H\phi_0) = (\psi|H\psi) = E$. In this system we consider
the initial vector $\psi' = \sqrt{p}\psi + \sqrt{1-p}\phi_0$, where $0 \leq p' \leq 1$. This $p'$ is precisely the
absorption parameter for the extended system. The time distribution does not change at all
since we defined it as normalized by $p'$. The energy expectation also does not change, but
$\Delta_\psi E^2 = p'\Delta_\psi E^2 + (1-p')(\Delta_\psi E)^2 = p'\Delta_\psi E^2$. Hence equations (5) and (6), which hold
with $p = 1$ for $\psi$, are equivalent to their versions for $\psi'$ with the factor $\sqrt{p'}$. More complex
ways in which the particle might not be seen by the detector are covered by the full proof.

From now on we just assume $p = 1$.

We will associate with any wavefunction $\psi \in \mathcal{H}$ another wavefunction $\hat{\psi}$, which is a
function of time, so that $|\psi(t)|^2$ is the arrival probability density. In other words, $\hat{\psi}$ is a
wavefunction in a time representation. For each $t$, $\psi(t)$ lies in the original Hilbert space $\mathcal{H}$.

We define $\hat{\psi} = J\psi$ with the linear operator

$$
(J\psi)(t) = \begin{cases} \sqrt{2\pi}D^{1/2}B_t\psi & \text{if } t \geq 0 \\ 0 & \text{otherwise} \end{cases},
$$

(8)

where the square root of the positive operator $D$ is taken in the operator sense. Then, for $t \geq 0$,

$$
\|(J\psi)(t)\|^2 = \frac{2}{\hbar} (B_t\psi|DB_t\psi) = -\frac{d}{dt} (B_t\psi|B_t\psi) = \mathbb{P}(t).
$$

(9)

Here we used the assumption that $p = 1$ for all states, so the normalizing factor $p$ in
equation (2) can be omitted. Equivalently, $J^*J = 1$. We denote by $\hat{T}$ the self-adjoint
operator of multiplication by $t$. Then the required moments of $\mathbb{P}(t)$ are $(T) = (\hat{T}\hat{T}\hat{\psi})$
and $(T^2) = (\hat{T}^2\hat{\psi})$.

The translation in the time representation is generated by the operator $\hat{H} = i\hbar d/dt$. By
differentiating equation (8) and using the assumption $H\hat{\psi} = K\psi$, we find, for $t \geq 0$,

$$
(\hat{H}J\psi)(t) = i\hbar\sqrt{2\pi}D^{1/2}B_t(-iK/\hbar)\psi = (JK\psi)(t) = (JH\psi)(t).
$$

(10)

This obviously also holds for $t < 0$. At $t = 0$ the definition equation (8) would appear to
allow a jump discontinuity, leading to a $\delta(t)$ contribution in equation (10). But since $D\psi = 0$
we also have $(J\psi)(0) = 0$, and hence there is no jump. We can thus take equation (10) as
an equation for functions, i.e. $\hat{H}\hat{\psi} = \hat{H}\psi = JH\psi$. Therefore, using $J^*J = 1$, the variances
$\Delta_\psi E^2 = \|H\psi\|^2 - (\psi|H\psi)^2$ and the corresponding $\Delta_\hat{\psi} E^2 = \|\hat{H}\hat{\psi}\|^2 - (\psi|\hat{H}\hat{\psi})^2$ are the same.
The time–energy uncertainty relation equation (5) thus follows from the standard position–
momentum one, applied to ‘position’ $\hat{T}$ and ‘momentum’ $\hat{H}$.

It is well-known that the uncertainty relation can be derived from the operator inequality
$\hat{H}^2 + \hat{T}^2 \geq 1$ and a dimensional scaling relation. A similar argument applied to wavefunctions
only on the positive time axis, using the inequality $\hat{H}^2 + \hat{T} \geq \lambda I$ gives equation (6). $\lambda$ in
this equation is determined from the ground state problem of a particle in a linear potential in
front of a wall, which is solved in terms of the Airy function. Using the gap to the first excited
state in this problem (and the oscillator Hamiltonian) gives the estimates for near-equality
equation (7).
5. Emission from a two-level system

Let us consider the simplest possible system to which the relations (5) and (6) apply. Unlike the covariant observable approach, in which the spectrum of $H$ has to be continuous, finite dimensional systems are included. We consider a two-level system with

$$H = \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega \\ \Omega & 0 \end{pmatrix}, \quad D = \frac{\hbar}{2} \begin{pmatrix} 0 & 0 \\ 0 & \gamma \end{pmatrix},$$

(11)

where $\Omega, \gamma > 0$ are parameters. The relevant quantity is $\gamma/\Omega$, since we could make $\Omega/2 = \hbar = 1$ by a choice of units. As the initial state we take $\psi = (1, 0)^T$, so our basic assumption $H\psi = (0, \hbar \Omega/2)^T = (H - iD)\psi = K\psi$ is satisfied. Obviously, $\langle H \rangle = 0$ and $\langle H^2 \rangle = \frac{\hbar^2}{2} \Omega^2$, so $\Delta E = \frac{\hbar}{\sqrt{2}} \Omega$.

One can explicitly exponentiate $B_t = \exp(-iKt/\hbar)$, and hence compute the probability density $P(t)$. The result is shown in figure 1. The moments are also readily calculated. Both $\langle T \rangle$ and $\Delta T$ attain their minimum when $\gamma = \sqrt{2}\Omega$. Then the uncertainty inequalities are satisfied as $1/\sqrt{2} \approx 0.707 > 0.500$ for equation (5), and $\sqrt{2} \approx 1.414 > 1.376$ for equation (6), so $\langle T \rangle \Delta E$ reaches the minimum to within 3%! This implies by equation (7) that the arrival time distribution $P(t)$ must be close to $P_{\text{min}}(t)$. The comparison is shown in figure 1.

6. Experimental implementation

Instances of the uncertainty inequality as such are not an interesting experimental target, since it is impossible not to implement it. On the other hand, instances with near minimal uncertainty can be a challenge. The two-level scheme approximations described above naturally arise in quantum optics when looking at an atom interacting with lasers. A feasible level scheme is the one of a single $^{40}\text{Ca}^+$ atom (similar level schemes exist in other atoms), trapped in a Paul trap, which is shown in figure 2. The transitions $1 \rightarrow 2$ and $2 \rightarrow 3$ are driven by on-resonance lasers resulting in Rabi-frequencies $\Omega_{12}$, resp. $\Omega_{23}$. The narrow quadrupole transition $1 \rightarrow 2$ can be frequency resolved by a narrow-linewidth laser, whereas the $2 \rightarrow 3$ transition is selected by choosing $\sigma$-polarized light. If $|\Omega_{23}| \ll \Gamma_{3\rightarrow 4}$, we will get approximately an efficient decay rate $\gamma = |\Omega_{23}|^2/\Gamma_{3\rightarrow 4}$ for level 2. If we consider only levels 1 and 2, the corresponding effective Hamiltonian, within the rotating wave approximation and in the interaction picture to get rid of any time dependence, will be $K = H - iD$ as in equation (11), with this $\gamma$ and $\Omega = \Omega_{12}$.
The initial level 1 can be efficiently prepared via optical pumping. The arrival time in state 2 is then measured by measuring the time of the first spontaneously emitted photon on the \(3 \rightarrow 4\) transition. In the proposed scheme, the total absorption probability \(p\) is smaller than 1 due to spontaneous scattering events from state 3 back to state 2. However, these events are suppressed by more than a factor of 200 due to favorable branching ratios and small Clebsch–Gordan coefficients on the \(2 \rightarrow 3\) transition. All other spontaneous decay channels result merely in reduced detection efficiency and do not affect the uncertainty relation. A typical Rabi frequency of \(\Omega_{12} \sim 2\pi \times 100\) kHz would require an easily achievable \(\Omega_{23} \sim 2\pi \times 1.73\) MHz to reach approximately the minimum of the product \(\langle T \rangle \Delta E\), see figure 1. The required time resolution for the photon detector in this scenario is on the order of a few ns, well within reach of current technology. Alternative implementations include vacuum-stimulated Raman transitions in an atom strongly coupled to a leaky cavity [19].

7. Outlook

The approach given here can be applied to other situations involving time in quantum mechanics, such as tunneling and decay scenarios. A standard detector model for such applications is the pointlike counter, formally given by \(D = \lambda \delta(x)\). In the finite dimensional \((n > 2)\) setting it remains an interesting problem to characterize the arrival time densities \(P(t)\), which can be engineered by a suitable choice of laser couplings and initial states.

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Appendix. Proof

The formal proof of the statements in the paper follows the sketch given there, with the following main differences.

- The operators $K$ and $H$ are allowed to be unbounded, and domain questions are treated explicitly. This covers cases where $K - H$ is not meaningful as an operator (e.g., a $\delta$-function potential). Therefore, the difference $D = i(K - H)$ appears nowhere, and the dilation operator $J$ has to be defined differently from (8).
- There is no assumption of total absorption, i.e. $p < 1$ is allowed.
- The differentiation (10) is only carried out under suitable scalar products, avoiding the discussion of distributional derivatives.
- We set $\hbar = 1$ for notational convenience.

A.1. The dilation

We begin by recapitulating the dilation construction from [15]. Since $B_t$ is a contraction semigroup, $-\frac{d}{dt} (B_t \psi | B_t \phi)$ is a positive semidefinite sesquilinear form on $\text{dom } K$. We denote its completion by $\hat{E}$, which we call the exit space, and by $j : \text{dom } K \rightarrow \hat{E}$ the embedding map, so that for $\phi, \psi \in \text{dom } K$:

$$\langle j\psi | j\phi \rangle_{\hat{E}} = -\frac{d}{dt} (B_t \psi | B_t \phi)_{t=0} = i(\langle \psi | K \phi \rangle - \langle K \psi | \phi \rangle).$$

(A.1)

The basic dilation operator $J$ maps into the space

$$\hat{\mathcal{H}} = L^2(\mathbb{R}, dt; \mathcal{E}),$$

(A.2)

which is the space of `$\mathcal{E}$-valued wavefunctions’ $t \mapsto \Psi(t) \in \mathcal{E}$ such that $\|\Psi\|^2 = \int_{\infty}^{\infty} \|\Psi(t)\|_2^2 < \infty$. For $\psi \in \text{dom } K$, we define

$$J(\psi)(t) = \begin{cases} j(B_t \psi) & \text{if } t \geq 0 \\ 0 & \text{if } t < 0 \end{cases}.$$  

(A.3)

Then

$$\|J\psi\|^2 = \int_0^{\infty} dt \langle jB_t \psi | jB_t \psi \rangle = \int_0^{\infty} dt \left( -\frac{d}{dt} (B_t \psi | B_t \psi) \right)$$

(A.4)

$$= -\|B_t \psi\|^2_{t=0} = \langle \psi | (\mathbb{I} - R) \psi \rangle,$$

(A.5)

where $R = \lim_{t \to \infty} B_t^* B_t$.

Hence $\|J\psi\| \leq \|\psi\|$, and $J$ extends by continuity to a unique operator $J : \mathcal{H} \rightarrow L^2(\mathbb{R}, dt; \mathcal{E})$, which we will denote by the same letter.

A.2. Time distributions

Now in the dilation space $\hat{\mathcal{H}}$ we have a time operator $\hat{T}$, which acts by multiplication with $t$. Its spectral projections $\hat{F}(\{t,s\})$ are a dilation of the arrival time observable $F$. That is, in analogy with equation (A.4) we get, for $0 < t < s$ and $\phi, \psi \in \text{dom } K$:

$$\langle J\phi | \hat{F}(\{t,s\}) J\psi \rangle = \int_t^s d\tau \langle jB_{\tau} \phi | jB_{\tau} \psi \rangle = -\langle B_t \phi | B_s \psi \rangle |_{\tau=t}^{\tau=s} = \langle \phi | F(\{t,s\}) \psi \rangle.$$  

(A.6)
Again, these expressions are directly verified on \( \text{dom} \ H \) and normalized, because \( J^*J = \mathbb{1} - R \), so \( p = \langle \psi | J^*J \psi \rangle \).

### A.3. Energy distributions

The dilated energy operator \( \hat{H} \) is defined as the generator of the translations \( \hat{U}_t = \exp(-i\hat{H}t) \), where

\[
(\hat{U}_t \psi)(t) = \Psi(t + \tau)
\]

for \( t, \tau \in \mathbb{R} \). Obviously, for \( t, \tau \geq 0 \) and \( \psi \in \text{dom} \ K \), we have \( (\hat{U}_t \psi)(t) = j(B_t \tau \psi) = (J B_t \psi)(t) \), and hence \( J^* \hat{U}_t J = J^* J B_t \). By taking adjoints we also get an expression for \( t < 0 \). To summarize,

\[
J^* \hat{U}_t J = \begin{cases} (\mathbb{1} - R)B_t & \text{if } t \geq 0 \\ B_t^*(\mathbb{1} - R) & \text{if } t \leq 0 \end{cases}.
\]

Again, these expressions are directly verified on \( \text{dom} \ K \) and extended by continuity to all of \( \mathcal{H} \). This shows that in the special case \( R = 0 \), \( \hat{U} \) is a dilation of the semigroup \( B_t \) in the sense of Szőkefalvi-Nagy et al. [20] and Davies [21]. Since \( B_t^* R B_t = R \), we can commute generators and \( R \) in the sense that

\[
R \text{ dom } K \subset \text{ dom } K^* \subset R K.
\]

The \( \hat{H} \)-distribution with respect to \( \hat{\psi} \) from equation (A.8) is the measure \( \langle \hat{\psi} | \hat{E}(d\omega) \hat{\psi} \rangle \), where \( \hat{E} \) is the spectral measure of \( \hat{H} \). The characteristic function (Fourier transform) of this distribution is

\[
C(t) = \int_{-\infty}^{\infty} e^{-i\omega t} \langle \hat{\psi} | \hat{E}(d\omega) \hat{\psi} \rangle = \langle \hat{\psi} | \hat{U}_t \hat{\psi} \rangle = \frac{1}{p} \langle \psi | J^* \hat{U}_t J \psi \rangle,
\]

which can be evaluated further using equation (A.10). The moments of the \( \hat{H} \)-distribution are obtained by differentiating \( C \) at zero. In general, of course, the piecewise defined function equation (A.10) is not differentiable at zero. However, with our assumption on \( \psi \), we can establish that the right and left derivatives coincide.

The conditions \( \psi \in \text{dom} \ K \cap \text{dom} \ H \) and \( K^* \psi = H \psi \) imply that \( \|j(\psi)\|^2 = i(\langle \psi | H \psi \rangle - \langle H \psi | \psi \rangle) = 0 \), so \( j \psi = 0 \) for such \( \psi \). Moreover, for all \( \phi \in \text{dom} \ K \),

\[
\langle \psi | K \phi \rangle - \langle K \psi | \phi \rangle = -i j(\psi \mid j \phi) = 0,
\]

whence \( K^* \psi = K \psi = H \psi \). Now the first derivative of the characteristic function becomes

\[
\text{i} p C'(0) = \begin{cases} \langle \psi | (\mathbb{1} - R)K \psi \rangle & \text{for } t = 0^+ \\ \langle \psi | K^* (\mathbb{1} - R) \psi \rangle & \text{for } t = 0^- \\ = \langle \psi | (\mathbb{1} - R)H \psi \rangle = \langle H \psi | (\mathbb{1} - R) \psi \rangle. \end{cases}
\]

Similarly, for the second order, and with the additional property \( \psi \in \text{dom} \ K^2 \), we get

\[
- p C''(0) = \begin{cases} \langle \psi | (\mathbb{1} - R)K^2 \psi \rangle & \text{for } t = 0^+ \\ \langle \psi | (K^*)^2 (\mathbb{1} - R) \psi \rangle & \text{for } t = 0^- \\ = \langle H \psi | (\mathbb{1} - R)H \psi \rangle. \end{cases}
\]
Hence, with $\lambda = \langle \psi | H | \psi \rangle$ we get the variance
\[
(\Delta E)^2 = \langle (H - \lambda 1) | (H - \lambda 1) | \psi \rangle \\
\geq \langle (H - \lambda 1) | (1 - R) (H - \lambda 1) | \psi \rangle \\
= p (-C''(0) - 2i\lambda C'(0) + \lambda^2 C(0)) \\
= p \int (\omega - \lambda)^2 \text{tr}(\hat{\psi} | \hat{E}(\omega) \hat{\psi}) \\
\geq p \min \lambda \int (\omega - \lambda)^2 \text{tr}(\hat{\psi} | \hat{E}(\omega) \hat{\psi}) \\
= p (\Delta H)^2.
\]

To summarize
\[
\Delta E \geq \sqrt{p} \Delta \hat{H}.
\] (A.16)

In particular, $\Delta E \Delta T \geq \sqrt{p} \Delta \hat{H} \Delta \hat{T} \geq \sqrt{p} / 2$, which proves equation (5). However, since we also want equation (6) and the error estimate equation (7), we need a more detailed analysis.

A.4. Conversion to ground state problems

The inequalities (5) and (6) are for a product of moments. It is advantageous to turn this into inequalities for the expectations of a sum of operators. For this we use a standard trick, which basically amounts to a dimensional analysis, and hence assures that we estimate quantities of the physical dimension time $\times$ energy. If we change the unit of time, we transform $\hat{T} \mapsto \eta^{-1} \hat{T}$, and $\hat{H} \mapsto \eta \hat{H}$. This change is also implemented by a unitary operator in $\hat{H}$. Similarly, we can shift $\hat{H}$ and $\hat{\tau}$ by multiples of the identity with unitary operators. This is the idea behind choosing the operators
\[
X = \eta^2 (\hat{H} - \epsilon)^2 + \eta^{-2} (\hat{T} - \tau)^2, \\
Y = \eta^2 (\hat{H} - \epsilon)^2 + \eta^{-1} \hat{\tau},
\] (A.17) (A.18)

where $Y$ is considered as a quadratic form on the subspace of functions vanishing for $t < 0$. These are just standard Schrödinger operators with $\hat{H}$ interpreted as the momentum and $\hat{T}$ as the position. In this guise they are well-known: $X$ is the Hamiltonian of the harmonic oscillator, and $Y$ describes a particle in a linear potential in front of a wall. Here the quadratic form point of view is dictated by our aim to bound the expectation value $\langle \hat{\psi} | Y | \hat{\psi} \rangle$ for functions in the positive-time subspace, and corresponds in operator theoretic terms to taking the Dirichlet boundary condition at $t = 0$. Note that this also corresponds to our discussion preceding equation (A.14), which says that for the initial vectors $\psi$ satisfying our assumptions, we have $j \psi = \hat{\psi}(0) = 0$. Both operators have purely discrete spectrum, because the potentials diverge at infinity. Moreover, the eigenvalues do not depend on the parameters $\tau, \epsilon, \eta$, because of the unitary equivalence. To compute the bottom eigenvalue, we can thus set $\epsilon = 0, \eta = 1$. For $X$ we have the eigenvalues $x_n = (2n + 1)$ (note that we left out a conventional factor of $1/2$ from the definition of the oscillator Hamiltonian). The ground state is, of course, a Gaussian.

The eigenvalue equation for $Y$ becomes the differential equation
\[
- \psi''(t) + t \psi(t) = y \psi(t),
\] (A.19)

which is solved in terms of the Airy function $\text{Ai}$ by
\[
\psi(t) = \text{Ai}(t - y).
\] (A.20)
Indeed, $A_i$ is defined to be that solution of $-A_i''(t) + t A_i(t) = 0$, which is square integrable at $t \to +\infty$. The eigenvalue equation comes out of the boundary condition: we must have $\psi(0) = A_i(0 - y) = 0$, i.e. $(−y)$ must be a zero of $A_i$ on the negative half-axis. These zeros are well-known and tabulated [22, table 9.9.1]. The first two are

\begin{align}
Z_1 &= -y_0 = -2.338\,1074\,104, \\
Z_2 &= -y_1 = -4.087\,9494\,441.
\end{align}

To get inequality equation (5) we choose $\varepsilon = \langle \hat{\psi} | \hat{H} \hat{\psi} \rangle$ and $\tau = \langle \hat{T} \rangle$. Taking expectations of the inequality $X \geq x_0^1$ we find

$$\eta^2 \Delta \hat{H}^2 + \eta^{-2} \Delta \hat{T}^2 \geq x_0 = 1.$$  \hfill (A.23)

Minimizing this expression over $\eta$, i.e. setting $\eta^2 = \Delta \hat{T} / \Delta \hat{H}$, we get $2 \Delta \hat{T} \Delta \hat{H} \geq 1$ for the canonical pair $\hat{T}, \hat{H}$, and equation (5) as stated by using equation (A.16). We went through this well-known argument just to stress the analogy with the proof of equation (6), for which the corresponding expression using $Y$ reads

$$\eta^2 \Delta \hat{H}^2 + \eta^{-1} \langle \hat{T} \rangle \geq y_0.$$  \hfill (A.24)

This time the minimum is attained at $\eta^2 = \langle \hat{T} \rangle / (2 \Delta \hat{H}^2)$, giving

$$3 \left( \frac{\langle T \rangle \Delta \hat{H}}{2} \right)^{\frac{1}{2}} \geq y_0.$$  \hfill (A.25)

Together with equation (A.16) this gives equation (6). It now remains to show equation (7) for the almost minimal case. For this we have to first provide an elementary estimate, which quantitatively captures the heuristic idea that in a gapped ground state problem only states close to the ground state can have expectations close to the bottom eigenvalue.

**A.5. Lemma on gapped ground states**

Let $A$ be an operator, which has a lowest, non-degenerate eigenvalue $a_0$ with normalized eigenfunction $\phi_0$, so that the rest of the spectrum lies in the half-axis $[a_1, \infty)$ with gap $a_1 - a_0 > 0$. That is, we can write

$$A = a_0 |\phi_0\rangle \langle \phi_0| + A_1$$  \hfill (A.26)

with

$$A_1 \geq a_1 (1 - |\phi_0\rangle \langle \phi_0|).$$

Now suppose that for some state $\rho$ we have

$$\text{tr} \, \rho A \leq a_0 + \alpha,$$  \hfill (A.28)

where $\alpha > 0$. Then we claim that

$$\| \rho - |\phi_0\rangle \langle \phi_0| \|_1 \leq 2 \sqrt{\frac{\alpha}{a_1 - a_0}},$$  \hfill (A.29)

where $\|X\|_1 = \text{tr} \sqrt{X^*X}$ denotes the trace norm of the operator $X$. The reason to write this in terms of density operators and trace norms (although we only need the case of a pure state $\rho = |\hat{\psi}\rangle \langle \hat{\psi}|$ later on) is that in this form it is clearer that the bound is equivalent to

$$|\text{tr}(\rho S) - |\phi_0\rangle \langle S |\phi_0| | \leq 2 \sqrt{\frac{\alpha}{a_1 - a_0}}.$$  \hfill (A.30)
for all operators $S$ with $\|S\| \leq 1$. Note that for any two density operators we have $\|\rho_1 - \rho_2\| \leq 2$. Hence the bound trivializes for $\alpha \geq a_1 - a_0$, but gives some information as long as the expectation $a_0 + \alpha$ lies in the gap.

For the proof we evaluate the inequality
\[
A \geq a_1 - (a_1 - a_0)\langle \phi_0 | \rho \phi_0 \rangle
\]
with $\rho$, getting
\[
a_0 + \alpha \geq \text{tr} \rho A \geq a_1 - (a_1 - a_0)\langle \phi_0 | \rho \phi_0 \rangle,
\]
which amounts to an estimate for the fidelity $\langle \phi_0 | \rho \phi_0 \rangle$, namely
\[
1 - \langle \phi_0 | \rho \phi_0 \rangle \leq \frac{\alpha}{a_1 - a_0}.
\] (A.31)

The trace norm estimate follows from this by [23, lemma 4.1].

### A.6. Almost minimal case

Let us begin with the variance inequality. Of course, it is a standard exercise in almost every quantum physics textbook to show that the uncertainty relation holds with equality exactly for Gaussians. Much less well-known is the stability statement for this minimal case, which we prove here. It makes an almost equally simple exercise, so one might have expected to see it posed in quantum mechanics courses the world over. However, we could not find a reference for it.

So suppose that $\Delta T \Delta E \leq (1 + \epsilon)\sqrt{p}/2$. By equation (A.16) this implies $2\Delta T \Delta \hat{H} \leq (1 + \epsilon)c$. The left-hand side of this inequality is just the expectation of $X$ with the minimizing choices of constants. Hence the assumption equation (A.28) is satisfied and the estimate equation (A.30) applies, which gives
\[
| \text{tr}(\rho S) - \langle \phi_0 | S \phi_0 \rangle | \leq 2 \sqrt{\frac{\epsilon}{x_1 - x_0}} = \sqrt{2\epsilon}
\] (A.32)
for any $S$ with $\|S\| \leq 1$. We choose $S$ as the multiplication operator with $s(t) = \text{sign}(\mathcal{P}(t) - \mathcal{P}_{\min}(t))$. Then
\[
\|\mathcal{P} - \mathcal{P}_{\min}\|_1 = \int_0^\infty \text{dt} | \mathcal{P}(t) - \mathcal{P}_{\min}(t) | = \int_0^\infty \text{dt} s(t)(\mathcal{P}(t) - \mathcal{P}_{\min}(t)) \leq \sqrt{2\epsilon}.
\] (A.33)

The argument for near equality of equation (6) is completely analogous. Suppose that $\langle T \Delta E \leq (1 + \epsilon)c\sqrt{p}$, so $\langle T \Delta \hat{H} \leq (1 + \epsilon)c$. Then the expectation of $Y$, which is the left-hand side of equation (A.25), is by a factor $(1 + \epsilon)^{2/3}$ larger than the absolute minimum. We can hence apply the estimate with $\alpha = ((1 + \epsilon)^{2/3} - 1)y_0 \leq 2y_0\epsilon/3$, which gives
\[
\|\mathcal{P} - \mathcal{P}_{\min}\|_1 \leq \gamma \sqrt{\epsilon}
\] (A.34)

with $\gamma = 2\sqrt{\frac{2y_0}{3(y_1 - y_0)}} \approx 1.888$. (A.35)
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