Generalized Time-Energy Uncertainty Relations and Bounds on Life Times of Resonances

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A precise form of the quantum-mechanical time-energy uncertainty relation is derived. For any given initial state (density operator), time-dependent Hamiltonian, and subspace of reference states, it gives upper and lower bounds for the probability of finding the system in a state in that subspace at a later or earlier time. The bounds involve only the initial data, the energy uncertainty in the initial state, and the energy uncertainty in the reference subspace. They describe how fast the state enters or leaves the reference subspace. They are exact if, but not only if, the initial state or the projection onto the reference subspace commute with the Hamiltonian. The basic tool used in the proof is a simple inequality for expectation values of commutators which generalizes the usual uncertainty relation. By introducing suitable comparison dynamics (trial propagators), the bounds can be made arbitrarily tight. They represent a time-dependent variational principle, in terms of trial propagators, which provides explicit error estimates and reproduces the exact time evolution when one varies over all trial propagators. As illustrations, we derive accurate lower bounds on the escape time of a particle out of a potential well modelling a quantum dot, and the total time before which a He^+ ion moving in a uniform magnetic field loses its electron.

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1. INTRODUCTION

A basic challenge in quantum mechanics is to understand how time-dependent Schrödinger equations, innocently linear and first-order in time as they are, admit solutions exhibiting an incredibly rich variety of different behavior, ranging from free wave-packet propagation to complex diffraction phenomena, from the slow decay of metastable states to fast optical switching, from quantum beats to seemingly irreversible or chaotic behavior. The origin of such diverse behavior is the oscillatory nature of the time evolution and the superposition principle which, by constructive and destructive interference, can produce virtually any “signal” (depending on the initial state and the Hamiltonian). A noteworthy example exhibiting many of these phenomena governed by a single Hamiltonian is the Jaynes-Cummings model [1], a prototype of two interacting quantum systems. The model produces collapses and revivals of the atomic population inversion, dynamic generation of approximate product states (disentanglement), irreversible subdynamics, and spontaneously broken symmetries [2-9].

The oscillatory nature of the quantum-mechanical time evolution is the source of various difficulties encountered when one attempts to solve the Schrödinger equation numerically. Reliable numerical methods to integrate the time-dependent Schrödinger equation for systems with several spatial variables have become available only quite recently [10,11]. They have been spurred by the development of very short and intense laser pulses (10^{-14} s, 10^{18} W/cm²) so as to provide a computational basis for the new processes driven or probed by such laser fields [11]. But even with these advances, the systems for which reliable calculations can be carried out and the times up to which the results are accurate remain limited. This is in contrast to the situation for stationary states where there are many methods to obtain accurate approximations. One may ask why similar methods do not exist for the time-dependent Schrödinger equation. The answer is that, just as for one real variable x the oscillatory function e^{ix} is more complicated to approximate numerically than the monotone decreasing function e^{-x} , it is much more difficult to estimate $e^{iHt/\hbar}$ than $e^{-\beta H}$ where H is the Hamiltonian. An estimation of $e^{-\beta H}$, for large β , is equivalent to estimating the low-lying eigenvalues $E_0 < E_1 < \dots$ and the corresponding eigenprojections $P_0, P_1, \dots$ of H , using that

$$e^{-\beta H} \sim e^{-\beta E_0} P_0 \tag{1a}$$

$$(e^{-\beta H} - e^{-\beta E_0} P_0) \sim e^{-\beta E_1} P_1, \dots \tag{1b}$$

as $\beta \rightarrow \infty$. A beautiful numerical implementation of (1) has recently been carried out to obtain high-precision eigenvalues and eigenmodes of a fractal drum [12,13]. Perhaps the most striking difference between $e^{-iHt/\hbar}$ and $e^{-\beta H}$ manifests itself in their path integral representations [14]: the Feynman integral for the propagator $e^{-iHt/\hbar}$ is an oscillatory integral with a generally somewhat dubious mathematical status; the Feynman-Kac integral for $e^{-\beta H}$ is given in terms of a positive, finite measure supported on Brownian paths.

Thus, it is of interest to ask whether quantitative information about the time evolution of states can be obtained, for example in the form of bounds analogous to those for stationary states, i.e., in the form of a variational principle, *without solving the Schrödinger equation*. In this paper we present a method that allows one to obtain such information under very general conditions.

The plan of the paper is as follows. In Sect. 2 we indicate, by means of selected examples, how results concerning time-dependent properties can be obtained without explicit knowledge of the propagator. The general theme illustrated in the examples is that knowledge of suitable properties of the spectral measure of the Hamiltonian in the initial state, such as its “energy spread”, sets limitations on how fast the state can change with time. For example, if the energy spread is small the system cannot depart rapidly from the initial state, or move rapidly into some final state. Conversely, if the state changes rapidly in time, the energy spread is necessarily large. We refer to a result of this type as a time-energy uncertainty relation. Sect. 2 serves to illustrate some ideas and illuminate goals we pursue in the sequel.

In Sects. 3 through 5 we derive the main result of the paper (Theorem 3). This result provides – for any given initial state (pure or mixed), any Hamiltonian (time-dependent or not), an arbitrary subspace of reference states, and any *guess* of an approximate propagator – explicit upper and lower bounds for the probability that the system is in a state belonging to the reference subspace at time t . The bounds have the following nice properties:

(i) Computationally, they only require expectations of quadratic expressions in the Hamiltonian, describing the energy uncertainty in the initial state or in the reference subspace. If the approximate (trial) propagator is nontrivial ($\neq$ unit operator) the Hamiltonian and the reference subspace enter the calculation of energy uncertainties in an appropriately transformed form.

(ii) The bounds are nontrivial even when the trial propagator is trivial, i.e., equals the unit operator (Theorem 2). In that case, the energy uncertainties quantify the degree

of noncommutativity of the Hamiltonian and the initial state, and of the Hamiltonian and the projection onto the reference subspace. This connection between uncertainty and noncommutativity is developed in Sect. 3 in a general form (Theorem 1). Our bounds in Theorem 2 describe what happens when neither the initial state nor the projection onto the subspace of final states are constants of motion. They coincide, i.e., simultaneously equal the exact result, if and only if the initial state or the projection is a constant of motion. They reproduce the exact result also in other instances.

(iii) The freedom to work with arbitrary trial propagators (as long as they define a differentiable family of unitary operators) offers the possibility to improve the bounds obtained from the trivial trial propagator in important ways. The upper and lower bounds coincide if the trial propagator equals the exact propagator. They provide a time-dependent variational principle that *includes error bars*. By restricting the reference subspace to be one-dimensional, restricting states to be pure and weakening the bounds, we obtain a time-dependent variational principle for wave functions with explicit error bars; (Corollary 1, Sect. 5).

In Sect. 6, we compare our results with earlier work. In particular, we describe precursors of Theorem 2. In the special case where the projection onto the reference subspace is one-dimensional and the initial state is pure, the bounds of Theorem 2 were previously obtained in [15]. We then contrast Theorem 3 with earlier time-dependent variational principles, e.g. with Spruch's bounds [16] which are sharpened and generalized in Theorem 3. Our bounds in Corollary 1 only require knowledge of a time-dependent family of states rather than of the trial propagator; a novel aspect of our methods. Finally, we draw some parallels between Theorem 3 and Nekhoroshev's method in classical mechanics [17].

Two specific applications of our general results are worked out in Sect. 7, illustrating the performance of a nontrivial trial propagator in Theorem 3. The trial propagator will be the propagator of a Hamiltonian (comparison dynamics), for which the time-dependent Schrödinger equation can be studied explicitly. The energy uncertainties to be evaluated are those of the Hamiltonian in the "interaction picture". The first example treats the escape to infinity (in arbitrary space dimensions) of an electron initially confined by a potential barrier. The second example analyzes how a one-electron ion on a circular classical orbit (induced, e.g., by a uniform magnetic field) loses its electron due to tidal effects. The effect is one of many consequences of the quantum-mechanical Larmor theorem recently proven in [18]. Both examples are instances of long-lived resonances (metastable

states). In both examples, we derive accurate lower bounds on life times. Our analysis also yields lower bounds on life times of atomic bound states when an external electric field is turned on.

2. ESTIMATES ON TIME EVOLUTION FROM SPECTRAL PROPERTIES: EXAMPLES

We consider a system described by a Hilbert space $\mathcal{H}$ of pure-state vectors and a family of time-dependent Hamiltonians H_t . Mixed states are represented by density operators ρ which are positive, trace-class operators on $\mathcal{H}$ of trace 1. A state at time t is denoted by ρ_t and is determined by the initial state ρ_0 by solving the Liouville equation

$$i\hbar\dot{\rho}_t = [H_t, \rho_t]. \quad (2a)$$

If the state ρ_0 is pure then $\rho_t = |\psi_t\rangle\langle\psi_t|$, where ψ_t solves the time-dependent Schrödinger equation

$$i\hbar\dot{\psi}_t = H_t\psi_t. \quad (2b)$$

In the following, we refer to both equations, (2a) and (2b), as the Schrödinger equation. Furthermore, we consider an orthogonal projection P ($P = P^* = P^2$) and denote the subspace onto which it projects by $P\mathcal{H}$. Our goal in this paper is to obtain bounds for the function

$$p_t := \text{tr}(P\rho_t) \quad (3)$$

which is the probability of finding the system in a state in the subspace $P\mathcal{H}$ at time t . Every experimental question about the time evolution can be cast in the form (3). For example, if we choose $p_t = |\psi_t\rangle\langle\psi_t|$ and $P = |\varphi\rangle\langle\varphi|$, then $p_t = |\langle\varphi|\psi_t\rangle|^2$, i.e., (3) gives the transition probability into some final state φ , or the survival probability of the initial state if $\varphi = \psi_0$. If the system consists of two subsystems and $P = P_I \otimes 1_{II}$, then (3) describes the probability of finding subsystem I in the subspace $P_I\mathcal{H}_I$. Thus, by a suitable choice of P and knowledge of p_t , we can track the state of the system as a function of time. One may think of P as a projection onto states of particular interest (“target” states), or as a state selector, or as a detector. We shall call it the reference projection, $P\mathcal{H}$ the reference subspace, and p_t the transition probability into the reference subspace.

As described in the introduction, we intend to use a time-energy uncertainty relation as a shortcut replacing an exact solution of (2). Our time-energy uncertainty relations do

not quite fit into the usual perspective which focusses attention on trying to find substitutes for the nonexistent “time operator” (see, e.g., [19-22]) or to find analogues of the position-momentum uncertainty relation by other means. Our uncertainty relations include several unconventional examples, but we leave out examples outside the framework of (3), such as delay times in scattering theory [20,23,24] and traversal times through potential barriers [25,26]. Two comprehensive reviews of time-energy uncertainty relations are refs. [19,27].

In this section, we specifically illustrate the general idea that information on the behavior of the probability p_t in t can be derived from properties of its Fourier transform, $\hat{p}_E$, of which its energy spread is but one example.

Example 1. A trivial situation where p_t can be calculated without solving (2) is when ρ_0 or P commutes with H_t for all $t \in [0, T]$. Then

$$p_t = p_0, \quad \text{for all } t \in [0, T]. \quad (4)$$

The proof, using e.g. the Trotter product formula for the propagator, is obvious. This example suggests that if ρ_0 or P almost commute with the Hamiltonians H_t , p_t should vary only slowly with t , and one ought to be able to estimate its variation in terms of the smallness of the commutator. This is the idea we shall make precise.

Example 2. A first step towards extending Example 1 to nonstationary states ρ_0 is the conventional time-energy uncertainty relation. It states that if the initial state is $\rho_0 = |\psi_0\rangle\langle\psi_0|$ and evolves under the time-independent Hamiltonian H , then

$$\tau_j \varepsilon_j \geq \hbar \gamma_j \quad (5)$$

where τ_j is one of several notions (labelled by j) of life time of the initial state, ε_j is the associated energy uncertainty, and γ_j is a constant. Eq. (5) is a version of the rule that the life time is inversely proportional to the energy width. We wish to quote five mathematically rigorous examples of inequalities of the form (5): They are the Mandelstam-Tamm inequality [23,24,28] ($j = 1$), two special cases of bounds obtained by Fleming [29] and Bhattacharyya [30] ($j = 2, 3$), the Gislason-Sabelli-Wood inequality [27] ($j = 4$), and Wigner’s inequality [31] ($j = 5$). In these examples, the life times are defined, respectively, by

$$\tau_1 := \inf_{\mathbf{1} \neq A = A^*, t} \frac{(\langle \psi_t | A^2 \psi_t \rangle - \langle \psi_t | A \psi_t \rangle^2)^{1/2}}{|(d/dt)\langle \psi_t | A \psi_t \rangle|}, \quad (6a)$$

$$\tau_2 := \inf \{t \geq 0 : |\langle \psi_0 | \psi_t \rangle|^2 = 1/2\}, \quad (6b)$$

$$\tau_3 := \inf \{t \geq 0 : |\langle \psi_0 | \psi_t \rangle|^2 = 0\}, \quad (6c)$$

$$\tau_4 := \int_0^\infty |\langle \psi_0 | \psi_t \rangle|^2 dt, \quad (6d)$$

$$\tau_5 := \min_{t_0} \left(\frac{\int_{-\infty}^\infty |\langle \varphi | \psi_t \rangle|^2 (t - t_0)^2 dt}{\int_{-\infty}^\infty |\langle \varphi | \psi_t \rangle|^2 dt} \right)^{1/2}. \quad (6e)$$

The energy uncertainties are given by

$$\varepsilon_j := (\langle \psi_0 | H^2 \psi_0 \rangle - \langle \psi_0 | H \psi_0 \rangle^2)^{1/2} \quad (j = 1, \dots, 4), \quad (7a)$$

$$\varepsilon_5 := \min_{E_0} \left(\frac{\int_{-\infty}^\infty |\langle \varphi | \delta(E - H) \psi_0 \rangle|^2 (E - E_0)^2 dE}{\int_{-\infty}^\infty |\langle \varphi | \delta(E - H) \psi_0 \rangle|^2 dE} \right)^{1/2}, \quad (7b)$$

and the constants (all of them optimal) are

$$\gamma_1 := 1/2, \quad (8a)$$

$$\gamma_2 := \pi/4, \quad (8b)$$

$$\gamma_3 := \pi/2, \quad (8c)$$

$$\gamma_4 := 3.5^{-3/2} \pi, \quad (8d)$$

$$\gamma_5 := 1/2. \quad (8e)$$

We first discuss the examples corresponding to $j = 1, \dots, 4$. In each of them ε_j is the usual definition of the uncertainty (standard deviation) of an observable, here of H , in the state ψ_0 . Thus each of them yields $\tau_j = \infty$ when ψ_0 is an eigenvector of H , in agreement with Example 1, and quantifies the magnitude of the commutator $[H, |\psi_0\rangle\langle\psi_0|]$ by

$$\varepsilon_j = \left\{ \frac{1}{2} \text{tr}(-[H, |\psi_0\rangle\langle\psi_0|]^2) \right\}^{1/2}, \quad (9)$$

for general ψ_0 . The equivalence of (7a) and (9) is verified by a simple computation. The time τ_1 is the time needed for the average of any observable A to be displaced by an amount equal to the standard deviation of A , i.e., it is the minimum time for ψ_t to change appreciably. The times τ_2 and τ_3 are the first half-life time and first death time of ψ_0 , respectively. The time τ_4 , being the integrated survival probability of ψ_0 , has the meaning

of an average life time of ψ_0 . None of these four inequalities makes any assumptions about the spectrum of H .

Wigner's inequality assumes that H has absolutely continuous spectrum and that an observer measuring φ watches the system (particle) pass. The time t_0 which minimizes $(\dots)^{1/2}$ in (6e) is the mean time of arrival at φ of the particle. Thus τ_5 is the spread in arrival time, i.e., the amount of time the particle spends in state φ . If H is the kinetic energy operator in d dimensions, then $|\langle \varphi | \psi_t \rangle|^2 \sim \text{const.} t^{-d}$, as $t \rightarrow \infty$, for generic initial conditions, in which case one has the trivial outcome $\tau_5 = \infty$ in $d \leq 3$. However, if one searches for ψ_0 and φ that minimize the product $\tau_5 \varepsilon_5$, it may be possible to identify resonance states, their life times, and energy widths for suitable H [31]. The energy distribution function in (7b) can be interpreted as follows: $|\langle \varphi | \delta(E - H) \psi_0 \rangle|^2 (dE)^2$ is the probability that the particle in state ψ_0 , if subjected to an energy measurement in the interval $(E, E + dE)$, can be detected at φ . Thus ε_5 is the width of the energy distribution that ψ_0 and φ have in common.

Example 3. A celebrated result which estimates (3), without solving (2), is Ruelle's theorem [32-34]. The system has the Hilbert space $L^2(\mathbb{R}^n)$ and a time-independent Hamiltonian of the form $H = \text{kinetic energy} + \text{potential}$. The initial state is $\rho_0 = |\psi_0\rangle\langle\psi_0|$ where ψ_0 is either in the subspace of bound states (spanned by the eigenvectors of H), or in the subspace of continuum states (orthogonal complement of the bound states). The theorem states that if in (3) we choose for P the projection P_r onto states with support in the ball $\{x \in \mathbb{R}^n : |x| < r\}$, for an arbitrary $r < \infty$, then

$$\lim_{r \rightarrow \infty} \inf_{t \geq 0} p_{r,t} = 1 \quad \text{if } \psi_0 \text{ is a bound state,} \quad (10a)$$

$$\lim_{t \rightarrow \infty} (1/t) \int_0^t p_{r,t'} dt' = 0, \quad \text{for any } r < \infty, \quad \text{if } \psi_0 \text{ is a continuum state.} \quad (10b)$$

Part (10a) says that an arbitrary superposition of stationary states (bound state) remains – with probability arbitrarily close to 1 – in some finite ball for all times. Part (10b) says that a wave packet of extended states leaves – with probability 1, when averaged over all times – every finite ball. The time average in (10b) comes into effect when the wave packet returns to the origin infinitely often, with increasingly long time intervals between returns, as may happen if the potential has increasingly distant bumps, producing singular continuous spectrum of H .

Let $d\mu_{\psi_0}/dE$ denote the inverse Fourier transform of the function $\langle \psi_0 | e^{-iHt/\hbar} \psi_0 \rangle$,

$$\langle \psi_0 | e^{-iHt/\hbar} \psi_0 \rangle = \int_{-\infty}^{\infty} e^{-iEt/\hbar} d\mu_{\psi_0}(E). \quad (11)$$

Clearly μ_{ψ_0} is a probability measure. The properties of μ_{ψ_0} invoked in Ruelle's theorem are slightly more refined than mere energy uncertainty. They concern the measure class of μ_{ψ_0} , while the usual energy uncertainty, eq. (7a), describes a crude global feature of μ_{ψ_0} (standard deviation). The results described in (10) illustrate the rule that the long-time behavior is governed by the fine structure of μ_{ψ_0} , while the short-time behavior is controlled by the coarse structure of μ_{ψ_0} . The results in *Example 2* provide short-time control. Different notions of slow vs. fast change therefore may require different properties of the measure μ_{ψ_0} . But whatever the property of μ_{ψ_0} is that is invoked, it typically requires far less information than knowledge of the exact propagator, or of the spectral decomposition of H . In the present example, we only need to know whether μ_{ψ_0} is atomic or non-atomic.

Example 4. Ruelle's theorem is remarkable because the reference subspaces it treats are infinite-dimensional and unrelated to the initial states. One expects that more detailed properties of the long-time behavior of p_t can be inferred if P in (3) is a low-dimensional projection related to the initial state. This is indeed the case: For general $\mathcal{H}$, arbitrary time-independent H , and $P = \rho_0 = |\psi_0\rangle\langle\psi_0|$, one has that

$$(1/t) \int_0^t p_{t'} dt' \geq \text{const.} t^{-D-\epsilon} \quad \text{for } t \rightarrow \infty, \quad \text{for arbitrary } \epsilon > 0, \quad (12)$$

where D is the fractal dimension (Hausdorff dimension) of the support of μ_{ψ_0} ; [35-37]. In (12), p_t is the survival probability of the initial state, $p_t = |\langle \psi_0 | \psi_t \rangle|^2$, and the result (12) says that the time-averaged survival probability cannot decay too fast. The case $D = 0$ corresponds to discrete point spectrum and implies a decay slower than any power law (in agreement with the fact that p_t is quasi-periodic in this case). It is the analogue of part (10a) in Ruelle's theorem. The case $0 < D < 1$ corresponds to a Cantor spectrum of Lebesgue measure zero; and $D = 1$ may correspond to absolutely continuous spectrum.

It is interesting to compare the hypotheses in (5), (10) and (12) in terms of what they assume about spectral measures, as described in Table I. The table shows that the conditions in Ruelle's theorem and in (12) differ in how they measure the size of two related sets. The decay (12) may be interpreted as resolving the case (10b) in Ruelle's theorem into corresponding subcases.

Example 5. As a final example for estimation of p_t from spectral properties, we mention the following obvious result: Let $\mathcal{H}$ be arbitrary, H a time-independent Hamiltonian bounded from below, $\rho_0 = |\psi_0\rangle\langle\psi_0|$, and P such that $p_0 = 0$ in (3). Then p_t either is nonzero on a dense open set of t values, or vanishes for all t , see e.g. [38]. This implies that if ρ_0 describes a source state of particles, and P is a detector separated from the source by an arbitrary distance, the detection probability p_t is nonzero immediately after $t = 0$. As pointed out in [39], this is not in conflict with Einstein causality.

Table I. Properties of the spectral measures μ_{ψ_0} and μ_{φ, ψ_0} invoked in *Examples 2/4*. The complex measure μ_{φ, ψ_0} is the one replacing μ_{ψ_0} if in (11) the left-hand side is replaced by $\langle\varphi|e^{-iHt/\hbar}\psi_0\rangle$.

Example	“Energy spread”	Determines
(7a)	$\min_{E_0} \left(\int_{-\infty}^{\infty} (E - E_0)^2 d\mu_{\psi_0}(E) \right)^{1/2}$	$\epsilon_j (j = 1, \dots, 4)$
(7b)	$\min_{E_0} \left(\frac{\int_{-\infty}^{\infty} (E - E_0)^2 \left \frac{d}{dE} \mu_{\varphi, \psi_0}(E) \right ^2 dE}{\int_{-\infty}^{\infty} \left \frac{d}{dE} \mu_{\varphi, \psi_0}(E) \right ^2 dE} \right)^{1/2}$	ϵ_5
(10)	μ_{ψ_0} atomic, or μ_{ψ_0} continuous	whether (10a) or (10b) applies
(12)	$\min\{\dim \Omega : \mu_{\psi_0}(\Omega) = 1, \Omega \text{ closed}\}$	D

3. INEQUALITIES FOR EXPECTATIONS OF COMMUTATORS

In this section we derive a trace inequality that will serve as our principal tool to generate upper and lower bounds for the probability p_t in (3). Since p_t satisfies

$$i\hbar p_t = \text{tr}(P[H_t, \rho_t]) = \text{tr}(\rho_t[P, H_t]) \quad (13)$$

by (2a) and (3), we seek bounds for expectations of the type $\text{tr}(iR[A, B])$ where R is a positive operator and A, B are selfadjoint. The starting point is the Schwarz inequality.

We use it in a form that will yield necessary and sufficient conditions for equality in the bounds:

Lemma 1. Let $(\cdot | \cdot)$ be a non-negative, sesquilinear form on a space of linear operators, i.e., satisfying $(A | B + C) = (A | B) + (A | C)$, $(A | bB) = b(A | B)$, $(A | B) = (B | A)^*$, and $(A | A) \geq 0$, for all operators A, B, C in its domain and all $b \in \mathbb{C}$. Then

$$|(A | B) - (B | A)|^2 \leq 4 |(A | B)|^2 \leq 4(A | A)(B | B). \quad (14)$$

Equality in the first part holds if and only if $\text{Re}(A | B) = 0$. Equality in the second part (Schwarz inequality) holds if and only if

$$(aA + ibB | aA + ibB) = 0, \quad \text{with} \quad (15)$$

$$(a, b) \neq (0, 0), \quad (16)$$

for some $a, b \in \mathbb{C}$. Simultaneous equality in both parts holds if and only if (15) and (16) are satisfied for some $a, b \in \mathbb{R}$.

Bounds for expectations of commutators are obtained from (14) by a suitable choice of the form $(\cdot | \cdot)$. One such inequality is the Heisenberg uncertainty relation:

Lemma 2 (Conventional uncertainty relation). Let ρ be a density operator and A, B selfadjoint operators. Then

$$|\text{tr}(\rho[A, B])|^2 \leq 4\{\text{tr}(\rho A^2) - \text{tr}^2(\rho A)\}\{\text{tr}(\rho B^2) - (\text{tr}^2(\rho B))\}. \quad (17)$$

Equality holds in (17) if and only if $\{a(A - \text{tr}(\rho A)) + ib(B - \text{tr}(\rho B))\}\rho = 0$, for some $a, b \in \mathbb{R}$, with $(a, b) \neq (0, 0)$. The right-hand side of (17) vanishes if and only if $A\rho = a\rho$ for some $a \in \mathbb{R}$, or $B\rho = b\rho$ for some $b \in \mathbb{R}$.

Proof. For general A and B , the form $(A | B) := \text{tr}(\rho A^* B)$ is a non-negative sesquilinear form. For selfadjoint A, B and real numbers a, b it satisfies

$$\begin{aligned} |\text{tr}(\rho[A, B])|^2 &= |(A - a | B - b) - (B - b | A - a)|^2 \\ &\leq 4(A - a | A - a)(B - b | B - b) \end{aligned} \quad (18)$$

by use of (14). Minimization of the bound (18) with respect to a and b , using $\text{tr}(\rho) = 1$, yields (17). The conditions for equality in (17) and for zero right-hand side of (17) follow

from Lemma 1, eq. (18), and the observation that $\text{tr}(\rho C^* C) = 0$ is equivalent to $C\rho = 0$ for arbitrary C . $\square$

The usual application of (17) is to estimate the standard deviations $\{\dots\}^{1/2}$ in terms of the expectation of the commutator. Our purpose, however, is the opposite: we wish to estimate the expectation of the commutator. Specifically, we seek a bound for the expectation of the commutator that equals zero if ρ commutes with A or B . The bound (17) does not have this property. The desired bound is achieved in the following two results. Their relation to the bound (17) will be discussed after Theorem 1.

Lemma 3 (Uncertainty relation for subspaces). Let P be an orthogonal projection and A, B selfadjoint operators. Then

$$|\text{tr}(P[A, B])|^2 \leq 4\text{tr}(PA^2 - PAPA) \text{tr}(PB^2 - PBPB). \quad (19)$$

Equality holds in (19) if and only if $[P, aA + ibB]P = 0$, for some real $(a, b) \neq (0, 0)$. The right-hand side of (19) vanishes if and only if $[P, A] = 0$ or $[P, B] = 0$.

Proof. For general A and B , we define

$$(A | B) := \text{tr}(PA^*(1 - P)BP) \quad (20a)$$

$$= \text{tr}(PA^*B - PA^*PB), \quad (20b)$$

where (20b) follows from $P = P^2$ and cyclic permutation under the trace. One easily verifies, using $P = P^2 = P^*$, that (20a) is a non-negative sesquilinear form. For selfadjoint A and B , it gives

$$\begin{aligned} (A | B) - (B | A) &= \text{tr}(PAB - PAPB - PBA + PBPA) \\ &= \text{tr}(P[A, B]) \end{aligned} \quad (21)$$

Substitution of (20) and (21) into (14) yields (19). Next, consider an arbitrary C such that $(C | C) = 0$. From (20) it follows that $\langle CP\psi | (1 - P)CP\psi \rangle = 0$, for all ψ . This implies $CP\psi \in P\mathcal{H}$ for all ψ , i.e., $CP = PCP$. Conversely, $CP = PCP$ implies $(C | C) = 0$. Thus $(C | C) = 0$ is equivalent to $[P, C]P = 0$, for general C , and equivalent to $[P, C] = 0$ for selfadjoint C . Together with Lemma 1, this proves the conditions for equality in (19) and for zero right-hand side of (19). $\square$

Theorem 1 (Strong uncertainty relation). Let R be a positive operator, $R \geq 0$, with pure point spectrum, eigenvalues $\{\lambda_n\}_{n=1}^N$, and corresponding eigenprojections $\{P_n\}_{n=1}^N$ ($N \leq \infty$). Furthermore, let A and B be self-adjoint operators. Then

$$| \operatorname{tr}(R[A, B]) |^2 \leq 4f^2(R, A) f^2(R, B), \quad (22)$$

where

$$f(R, A) := \left(\sum_{n=1}^N \lambda_n \operatorname{tr}(P_n A^2 - P_n A P_n A) \right)^{1/2}. \quad (23)$$

Equality holds in (22) if and only if $[R, aA + ibB]R = 0$, for some real $(a, b) \neq (0, 0)$. The right-hand side of (22) vanishes if and only if $[R, A] = 0$ or $[R, B] = 0$.

Proof. For general A and B , we define

$$(A | B) := \sum_{n=1}^N \lambda_n \operatorname{tr}(P_n A^*(1 - P_n) B P_n). \quad (24)$$

Just as for (20), one verifies that (24) is a non-negative sesquilinear form, and, for self-adjoint A, B , satisfies $(A | B) - (B | A) = \operatorname{tr}(R[A, B])$, which yields (22) from (14). The remaining assertions in Theorem 3 follow from Lemma 1 and the following. For arbitrary C , one has

$$(C | C) = 0 \Leftrightarrow CP_n = P_n CP_n, \quad \text{for all } n \quad (25a)$$

$$\Rightarrow [P_n, C]P_m = 0, \quad \text{for all } n, m \quad (25b)$$

$$\Rightarrow [R, C]R = 0 \quad (25c)$$

$$\Rightarrow \sum_n \lambda_n P_n CP_m - \lambda_m CP_m = 0, \quad \text{for all } m \quad (25d)$$

$$\Rightarrow P_m CP_m = CP_m, \quad \text{for all } m \quad (25e)$$

$$\Rightarrow (C | C) = 0. \quad (25f)$$

Part (25a) is clear from the proof of Lemma 3 and $\lambda_n > 0$, for all nonzero terms in (24). Parts (25b,c) follow from the spectral theorem. Multiplication of (25c) from the right by P_m yields (25d). Multiplication of (25d) from the left by P_n yields $(\lambda_n - \lambda_m)P_n CP_m = 0$ and hence $P_n CP_m = 0$ for $n \neq m$, which gives (25e) by substitution into (25d). The final step follows from (25a). This shows that $(C | C) = 0$ is equivalent to $[R, C]R = 0$, for general C , and equivalent to $[R, C] = 0$, for selfadjoint C . $\square$

Table II. Corollaries of Theorem 1. The table lists, for different cases of R , the resulting properties of the uncertainty $f(R, A)$ and of the bounds (17),(19),(22). The observable A is arbitrary. The expressions (26), $\dots$, (29) are all nonnegative.

	$f^2(R, A)$	Bounds
$R = \rho = \psi\rangle\langle\psi $	$= \text{tr}(\rho A^2 - \rho A \rho A) \quad (26a)$ $= \text{tr}(\rho A^2) - \text{tr}^2(\rho A) \quad (26b)$ $= \langle\psi A^2 \psi\rangle - \langle\psi A \psi\rangle^2 \quad (26c)$	(17),(19), and (22) coincide
$R = \rho = \rho^* \geq 0,$ $\text{tr}(\rho) = 1$	$\leq \text{tr}(\rho A^2) - \text{tr}^2(\rho A) \quad (27)$	(22) implies (17)
$R = P = P^* = P^2$	$= \text{tr}(P A^2 - P A P A) \quad (28a)$ $= (1/2)\text{tr}(-[P, A]^2) \quad (28b)$	(19) and (22) coincide
$R = \text{general, as}$ in Theorem 1	$\geq \text{tr}(R A^2 - \sqrt{R} A \sqrt{R} A) \quad (29a)$ $= (1/2)\text{tr}(-[\sqrt{R}, A]^2) \quad (29b)$	only (22) holds

We call the quantity $f(R, A)$ the uncertainty of the observable A with respect to the weight R . For a density operator ρ and an orthogonal projection P , we call $f(\rho, A)$ the uncertainty of A in state ρ and $f(P, A)$ the uncertainty of A in the subspace $P\mathcal{H}$. The relation of Theorem 1 to Lemma 2 and Lemma 3 is exhibited in Table II. The first line shows that the three uncertainty relations coincide for pure states. The second line shows that Theorem 1 is stronger than Lemma 2. The third line shows that Theorem 1 includes also Lemma 3. The last line will be discussed below. Of the statements in Table II, only (27) and (29) need proof. Inequality (27) follows from

$$f^2(\rho, A) = \text{tr}(\rho A^2) - \sum_n \lambda_n \text{tr}(P_n A P_n A), \quad (30)$$

$$\begin{aligned} \text{tr}^2(\rho A) &= \left(\sum_n \lambda_n \text{tr}(P_n P_n A P_n) \right)^2 \\ &\leq \left(\sum_n \lambda_n \sqrt{\text{tr}(P_n^2) \text{tr}((P_n A P_n)^2)} \right)^2 \end{aligned} \quad (31a)$$

$$\begin{aligned} &= \left(\sum_n \sqrt{\lambda_n \text{tr}(P_n)} \sqrt{\lambda_n \text{tr}((P_n A P_n)^2)} \right)^2 \\ &\leq \left(\sum_n \lambda_n \text{tr}(P_n) \right) \left(\sum_n \lambda_n \text{tr}((P_n A P_n)^2) \right) \end{aligned} \quad (31b)$$

$$= \sum_n \lambda_n \text{tr}(P_n A P_n A) \quad (31c)$$

where we have used the Schwarz inequality $|\text{tr}(X^* Y)| \leq \{\text{tr}(X^* X) \text{tr}(Y^* Y)\}^{1/2}$ in (31a), the Cauchy inequality in (31b), and $\text{tr}(\rho) = 1$ in (31c). Inequality (29) follows from

$$\begin{aligned} &f^2(R, A) - \text{tr}(R A^2 - \sqrt{R} A \sqrt{R} A) \\ &= \sum_{n,m} \sqrt{\lambda_n \lambda_m} \text{tr}(P_n A P_m A P_n) - \sum_n \lambda_n \text{tr}(P_n A P_n A P_n) \end{aligned} \quad (32)$$

and $\text{tr}(P_n A P_m A P_n) \geq 0$ for all n, m .

Thus, Theorem 1 sharpens and extends the conventional uncertainty relation in such a way that $f(R, A) = 0$ if and only if $[R, A] = 0$, i.e., that the uncertainty $f(R, A)$ is a measure of the noncommutativity of R and A . It decomposes the expectation of the commutator $[A, B]$ into a product of expectations involving A and B separately. The transformation properties

$$f(rR, aA) = r^{1/2} |a| f(R, A) \quad (33a)$$

$$f(R, U^* A U) = f(U R U^*, A) \quad (33b)$$

($r \geq 0; a \in \mathbb{R}; U = \text{unitary}$) ensure that both sides of (22) transform in the same way under rescaling and unitary transformation of the operators. For given observables A and B , the condition

$$[R, aA + ibB]R = 0, \quad a^2 + b^2 > 0 \quad \text{for some } a, b \in \mathbb{R} \quad (34)$$

defines the class of minimum-uncertainty weights R , i.e., the weights for which equality holds in (22). If A and B are position and momentum of a particle, and one chooses $R = |\psi\rangle\langle\psi|$, the condition (34) reduces to the familiar characterization of coherent states. Since the inequality (22) is tighter than (17), the class of weights obeying (34) is larger than the class of minimum-uncertainty states for (17), however. For example, the unit operator is always a minimum-uncertainty weight. More generally, every positive function of A or B with pure point spectrum is a minimum-uncertainty weight.

We close this section with two remarks about improvements of Theorem 1. The first concerns the question whether (22) can be improved by decomposing the eigenprojections P_n in (23) into lower-dimensional orthogonal projections (clearly, all that is needed for (22) to hold is that $R = \sum_n \lambda_n P_n$, $\lambda_n \geq 0$, and $P_n = P_n^* = P_n^2$). The answer is no. Indeed, if P , P' and P'' are orthogonal projections with $P = P' + P''$, then

$$f^2(P', A) + f^2(P'', A) - f^2(P, A) = 2\text{tr}(P'AP''AP') \geq 0. \quad (35)$$

The second question is whether (22) can be improved by replacing $f(R, A)$ by $\{\text{tr}(RA^2 - \sqrt{R}A\sqrt{R}A)\}^{1/2}$, as (28) and (29) in Table II seem to suggest. But simple 2×2 -matrices exist for which (22) is no longer valid when this replacement is made. Thus Theorem 1 appears to be optimal.

4. GENERALIZED TIME-ENERGY UNCERTAINTY RELATION

Our key idea is that Theorem 1, when applied to the equation of motion (13), separates the right-hand side of (13) into factors which, by the orthogonal projection property of P , yield closed-form differential inequalities for p_t . These inequalities can then be integrated. To treat the general case where the Hamiltonian is time-dependent, it is useful to first consider the probability p_t as a function of both the initial time and the final time.

Proposition 1. Let $U_{t,s}$ be the unitary propagator from initial time s to final time t , for a system with time-dependent Hamiltonian H_t at time t . It satisfies the equation

$$U_{t,s} = 1 - (i/\hbar) \int_s^t H_{t'} U_{t',s} dt' \quad (36)$$

for all $s, t \in \mathbb{R}$.¹ Let ρ_0 be a fixed density operator and P an orthogonal projection. Define

$$\rho_{t,s} := U_{t,s} \rho_0 U_{t,s}^* \quad (37)$$

$$p_{t,s} := \text{tr}(P \rho_{t,s}). \quad (38)$$

The operator $\rho_{t,s}$ and the function $p_{t,s}$ describe the evolution of the density operator ρ_0 from time s to time t (Schrödinger picture; $\rho_{s,s} = \rho_0$) and the corresponding expectation value of P , respectively. Then

$$\left| \frac{\partial}{\partial t} p_{t,s} \right| \leq 2\hbar^{-1} f(P, H_t) \sqrt{p_{t,s} - p_{t,s}^2} \quad (39a)$$

$$\left| \frac{\partial}{\partial s} p_{t,s} \right| \leq 2\hbar^{-1} f(\rho_0, H_s) \sqrt{p_{t,s} - p_{t,s}^2} \quad (39b)$$

for all $s, t \in \mathbb{R}$, where f is the function defined in eq. (23).

Proof. Equation (36) implies that the propagator satisfies $U_{s,t} = U_{t,s}^*$ and

$$i\hbar \frac{\partial}{\partial t} U_{t,s} = H_t U_{t,s}; \quad U_{s,s} = 1 \quad (40a)$$

$$i\hbar \frac{\partial}{\partial s} U_{t,s} = -U_{t,s} H_s; \quad U_{t,t} = 1. \quad (40b)$$

Differentiation of (37) with respect to t and s , together with eqs. (40a,b) and their adjoints, leads to

$$i\hbar \frac{\partial}{\partial t} \rho_{t,s} = [H_t, \rho_{t,s}] \quad (40a)$$

$$i\hbar \frac{\partial}{\partial s} \rho_{t,s} = -U_{t,s} [H_s, \rho_0] U_{t,s}^*. \quad (40b)$$

From eqs. (37), (40a) and Theorem 1, it follows that

$$\begin{aligned} \hbar \left| \frac{\partial}{\partial t} p_{t,s} \right| &= | \text{tr}(P [H_t, \rho_{t,s}]) | \\ &\leq 2f(P, H_t) f(P, \rho_{t,s}). \end{aligned} \quad (41)$$

For any orthogonal projection P and density operator ρ , one has the inequality

$$\begin{aligned} f^2(P, \rho) &= \text{tr}(P \rho (1 - P) \rho) \\ &= \text{tr}((\sqrt{\rho} P \sqrt{\rho})^* \sqrt{\rho} (1 - P) \sqrt{\rho}) \\ &\leq \{ \text{tr}((P \rho P)^2) \text{tr}(((1 - P) \rho (1 - P))^2) \}^{1/2} \\ &\leq \{ \text{tr}^2(P \rho P) \text{tr}^2((1 - P) \rho (1 - P)) \}^{1/2} \\ &= \text{tr}(P \rho) - \text{tr}^2(P \rho), \end{aligned} \quad (42)$$

¹It is necessary to specify some hypotheses on the domain of definition of the operators H_t and their dependence on t . Eq. (36) then holds on a dense subspace of the Hilbert space.

where we have used (23) in the first line, the Schwarz inequality $| \operatorname{tr}(X^*Y) | \leq \{ \operatorname{tr}(X^*X) \operatorname{tr}(Y^*Y) \}^{1/2}$ in the third line, and nonnegativity of the eigenvalues of $P\rho P$ and $(1-P)\rho(1-P)$ in the fourth line; (recall that $\operatorname{tr}\rho = 1$). Equality holds in (42) if ρ is a pure state. Combination of (41), (42), and (38) proves (39a).

From (37), (40b), and Theorem 1, it follows that

$$\begin{aligned} \hbar \left| \frac{\partial}{\partial s} p_{t,s} \right| &= | \operatorname{tr}(PU_{t,s}[H_s, \rho_0]U_{t,s}^*) | \\ &= | \operatorname{tr}(\rho_0[H_s, U_{t,s}^*PU_{t,s}]) | \\ &\leq 2f(\rho_0, H_s)f(\rho_0, U_{t,s}^*PU_{t,s}) \\ &= 2f(\rho_0, H_s)f(\rho_{t,s}, P) \\ &\leq 2f(\rho_0, H_s)\{ \operatorname{tr}(\rho_{t,s}P) - \operatorname{tr}^2(\rho_{t,s}P) \}^{1/2}. \end{aligned} \quad (43)$$

In the last two lines of (43), we have used (33b) and (27), (see Table II). Inequality (43), together with (38), proves (39b). $\square$

Proposition 2. If the Hamiltonians H_t and $H_{t'}$ in Proposition 1 commute, for all t and t' , then the bounds (39a,b) are also valid with the replacements

$$f(P, H_t) \mapsto \min\{f(P, H_t), f(\rho_0, H_t)\} \quad (44a)$$

$$f(\rho_0, H_s) \mapsto \min\{f(P, H_s), f(\rho_0, H_s)\}. \quad (44b)$$

Proof. By rewriting the equations of motion (40a,b) as

$$i\hbar \frac{\partial}{\partial t} \rho_{t,s} = U_{t,s}[\tilde{H}_{t,s}, \rho_0]U_{t,s}^* \quad (40a')$$

$$i\hbar \frac{\partial}{\partial s} \rho_{t,s} = -[\tilde{H}_{s,t}, \rho_{t,s}], \quad (40b')$$

where $\tilde{H}_{t,s} := U_{t,s}^* H_t U_{t,s}$ is the Hamiltonian in the Heisenberg picture, and proceeding as in Proposition 1, one obtains the alternative bounds

$$\begin{aligned} \hbar \left| \frac{\partial}{\partial t} p_{t,s} \right| &= | \operatorname{tr}(\rho_0[\tilde{H}_{t,s}, U_{t,s}^*PU_{t,s}]) | \\ &\leq 2f(\rho_0, \tilde{H}_{t,s})f(\rho_0, U_{t,s}^*PU_{t,s}) \\ &\leq 2f(\rho_0, \tilde{H}_{t,s})\sqrt{p_{t,s} - p_{t,s}^2}, \end{aligned} \quad (39a')$$

$$\begin{aligned} \hbar \left| \frac{\partial}{\partial s} p_{t,s} \right| &= | \operatorname{tr}(P[\tilde{H}_{s,t}, \rho_{t,s}]) | \\ &\leq 2f(P, \tilde{H}_{s,t})f(P, \rho_{t,s}) \\ &\leq 2f(P, \tilde{H}_{s,t})\sqrt{p_{t,s} - p_{t,s}^2}. \end{aligned} \quad (39b')$$

They are quite useless in general, because, unlike in Proposition 1, the factors $f(\dots, \dots)$ here involve the little known propagator $U_{t,s}$ via $\tilde{H}_{t,s}$. But if the Hamiltonians at different times commute, then $U_{t,s}$ commutes with H_t . In that case, one has $\tilde{H}_{t,s} = H_t$ and $\tilde{H}_{s,t} = H_s$, so that (39') competes with (39) and yields the improvement (44). $\square$

Proposition 3. Under the hypotheses of Proposition 1, the probability $p_{t,s}$ is bounded from above and below, for all $s, t \in \mathbb{R}$, by

$$p_{t,s} \stackrel{\leq}{\geq} \sin_*^2 \left(\arcsin \sqrt{\text{tr}(P\rho_0)} \pm \hbar^{-1} \min \left\{ \int_s^t f(P, H_\tau) d\tau, \int_s^t f(\rho_0, H_\sigma) d\sigma \right\} \right) \quad (45)$$

where, without loss of generality, we have assumed that $s < t$, and

$$\sin_*(x) := \begin{cases} 0 & \text{if } x \leq 0 \\ \sin x & \text{if } 0 \leq x \leq \pi/2 \\ 1 & \text{if } x \geq \pi/2. \end{cases} \quad (46)$$

Proof. From Proposition 1 we have the bounds

$$\pm \frac{\partial}{\partial \tau} p_{\tau,s} \leq 2\hbar^{-1} f(P, H_\tau) \sqrt{p_{\tau,s} - p_{\tau,s}^2} \quad (47)$$

$$\pm \frac{\partial}{\partial \sigma} p_{t,\sigma} \leq 2\hbar^{-1} f(\rho_0, H_\sigma) \sqrt{p_{t,\sigma} - p_{t,\sigma}^2}. \quad (48)$$

For $s < t$, integration of (47) by separation of variables, from $\tau = s$ to $\tau = t$, gives

$$\pm \int_{p_{s,s}}^{p_{t,s}} (p - p^2)^{-1/2} dp \leq 2\hbar^{-1} \int_s^t f(P, H_\tau) d\tau \quad \text{if } s < t, \quad (49)$$

where the integral on the left-hand side is well-defined because $0 \leq p_{s,t} \leq 1$. Integration of (48), from $\sigma = t$ to $\sigma = s$, gives

$$\pm \int_{p_{t,t}}^{p_{t,s}} (p - p^2)^{-1/2} dp \geq 2\hbar^{-1} \int_t^s f(\rho_0, H_\sigma) d\sigma. \quad (50)$$

The sense of inequality (50) is opposite to that of (49), because, in (50), we integrate in the negative σ -direction. Since $p_{s,s} = p_{t,t} = \text{tr}(P\rho_0)$, the two inequalities compete with each other and yield

$$\begin{aligned} \pm \int_{\text{tr}(P\rho_0)}^{p_{t,s}} (p - p^2)^{-1/2} dp &= \pm 2(\arcsin \sqrt{\text{tr}(P\rho_0)} - \arcsin \sqrt{p_{t,s}}) \\ &\leq 2\hbar^{-1} \min \left\{ \int_s^t f(P, H_\tau) d\tau, \int_s^t f(\rho_0, H_\sigma) d\sigma \right\}. \end{aligned} \quad (51)$$

Solving (51) for $\arcsin \sqrt{p_{t,s}}$ and applying the function $\sin_\star^2$ on both sides of the inequality, one obtains the result (45) by monotonicity of $\sin_\star$. (If $s > t$ the integration limits in (45) are interchanged.) $\square$

Proposition 3 explains why it is important to consider the two-point probability $p_{t,s}$ in Proposition 1: The rate of change of the probability in the forward time direction is bounded by the energy uncertainty in the subspace $P\mathcal{H}$ [eq. (39a)]. The rate of change in the backward time direction is bounded by the energy uncertainty in the initial state ρ_0 [eq. (39b)]. Hence if we want to obtain an inequality that combines the two energy uncertainties, we have to consider variation of both, the initial time s and the final time t . This is precisely what we have done in the proof of Proposition 3: The τ -integration of (47) is from left to right, but the σ -integration of (48) is from right to left.

We now return to the original situation in which the initial time is set equal to zero ($s = 0$). To further simplify expressions, we choose final times to be positive ($t \geq 0$), with the understanding that the opposite case ($t \leq 0$) is equally easy to get from Proposition 3. We then have the following theorem.

Theorem 2 (time-energy uncertainty relation). Consider a quantum-mechanical system with a family of time-dependent Hamiltonians H_t , in an initial state ρ_0 . Let P be an orthogonal projection, and $P\mathcal{H}$ a subspace of possible states of the system at time t . Then the probability p_t , defined in eq. (3), is bounded from above and below by

$$p_t \stackrel{\leq}{\geq} \sin_\star^2 \left(\arcsin \sqrt{p_0} \pm \hbar^{-1} \min \left\{ \int_0^t f(P, H_s) ds, \int_0^t f(\rho_0, H_s) ds \right\} \right) \quad (52)$$

for all $t \geq 0$. The functions f and $\sin_\star$ are defined in eqs. (23) and (46), respectively. In the special case that $[H_s, H_{s'}] = 0$, for all $0 \leq s, s' \leq t$, one has the improvement

$$p_t \stackrel{\leq}{\geq} \sin_\star^2 \left(\arcsin \sqrt{p_0} \pm \hbar^{-1} \int_0^t \min \left\{ f(P, H_s), f(\rho_0, H_s) \right\} ds \right). \quad (53)$$

The upper and lower bound in (52) coincide if and only if either $[P, H_s] = 0$, or $[\rho_0, H_s] = 0$, for all $0 \leq s \leq t$. The bounds (53) coincide if and only if, for all $0 \leq s \leq t$, either $[P, H_s] = 0$, or $[\rho_0, H_s] = 0$.

Proof. Inequality (52) is Proposition 3, specialized to zero initial time and positive final time. Inequality (53) follows from Proposition 2: One substitutes (44a) into (39a) and integrates in a way similar to the integration in Proposition 3. The conditions for the coincidence of upper and lower bounds are clear from Theorem 1. $\square$

Theorem 2 is the central result of this paper. It achieves the goals set out in Sects. 1 and 2 in the following way:

(i) The bounds (52) do not require any information about the propagator or the solution of the Schrödinger equation (2). All they require is the ability to compute the energy uncertainty in the reference subspace, $f(P, H_s)$, and the energy uncertainty in the initial state, $f(\rho_0, H_s)$. Since the energy uncertainties involve only expectations of quadratic expressions in H_s , eq. (23), their computation is easy, compared to the task of solving the Schrödinger equation. For example, if the Hamiltonian is an $N \times N$ -matrix, the calculation of $f(\dot{P}, H_s)$ requires three matrix multiplications [recall eq. (28)], i.e., $\approx 3N^2$ operations. Diagonalization of H_s , as a step to solve (2), requires $O(N^3)$ operations [35]. In the rare event that $f(P, H_s)$ or $f(\rho_0, H_s)$ are difficult to compute one may drop one of them from (52), or estimate $f(\rho_0, H_s)$ by using (27) (Table II), at the expense of obtaining weaker bounds for p_t . Difficulties in computing $f(P, H_s)$ or $f(\rho_0, H_s)$ may occur only if P or ρ_0 have infinite rank (large reference subspace or highly mixed state). In the other extreme, where P and ρ_0 have rank one, i.e., where $P = |\varphi\rangle\langle\varphi|$ and $\rho_0 = |\psi_0\rangle\langle\psi_0|$, one has

$$f(P, H_s) = (\langle\varphi|H_s^2\varphi\rangle - \langle\varphi|H_s\varphi\rangle^2)^{1/2} \quad (54a)$$

$$f(\rho_0, H_s) = (\langle\psi_0|H_s^2\psi_0\rangle - \langle\psi_0|H_s\psi_0\rangle^2)^{1/2} \quad (54b)$$

by eq. (26). In this case, the energy uncertainties are the usual standard deviations with respect to vector states and simple to estimate.

(ii) The bounds (52) express a time-energy uncertainty relation, because they manifestly imply that p_t remains close to its initial value p_0 (“large life time of ρ_0 ”) if the energy uncertainty in $P\mathcal{H}$ or ρ_0 is small. Conversely, they imply that the energy uncertainty in $P\mathcal{H}$ and the energy uncertainty in ρ_0 must be large if p_t departs rapidly from p_0 (“short life time of ρ_0 ”).

(iii) By the property that $f(R, H_s) = 0$ if and only if $[R, H_s] = 0$, the bounds (52) clearly relate the change of p_t to the degree of noncommutativity of the pairs (P, H_s) and (ρ_0, H_s) . They show that $p_t \equiv p_0$ if P or ρ_0 is a constant of motion. They generally show what happens if P and ρ_0 are close to constants of motion.

(iv) The bounds (52) are invariant with respect to the interchange of P and $1 - P$. That is, if we write $p_t = \text{tr}(P\rho_t)$ and $p'_t = \text{tr}((1 - P)\rho_t)$, then the upper bound for p_t gives the lower bound for p'_t and the lower bound for p_t gives the upper bound for p'_t . This

follows from the identity

$$\sin_*^2(\arcsin \sqrt{p_0} \pm x) = 1 - \sin_*^2(\arcsin \sqrt{1-p_0} \mp x).$$

It shows that the bounds naturally respect the complementary nature of the subspaces $P\mathcal{H}$ and $(1-P)\mathcal{H}$, and the associated probability interpretations of p_t and $1-p_t$. Variants of the bounds (52) are obtained by applying the inequalities

$$\sin_*(\arcsin \sqrt{p_0} \pm x) \stackrel{\leq}{\geq} \sqrt{p_0} + 2 \min\{\sqrt{1-p_0}, \pm 1\} \sin_*(x/2) \quad (55a)$$

$$\stackrel{\leq}{\geq} \sqrt{p_0} \pm x, \quad (55b)$$

for $x \geq 0$. We use (55a) and (55b) in Sects. 5 and 6.

(v) The bounds (52) depend on the energy uncertainties in $P\mathcal{H}$ and ρ_0 , integrated up to time t (cumulative uncertainties). Thus the bounds coincide at $t = 0$ and increasingly depart from each other as t increases. When the smaller of the two cumulative uncertainties reaches the value $\hbar(\pi/2 - \arcsin \sqrt{p_0})$ or $\hbar \arcsin \sqrt{p_0}$, the upper or lower bound for p_t becomes trivial, i.e., 1 and 0, respectively. For example, if $p_0 = 1$, the upper bound is trivial at all times; and if $p_0 = 0$, the lower bound is trivial at all times. This behavior as a function of t shows that the bounds (52) control the short-time behavior of p_t , in agreement with the fact that uncertainties $f(P, H_s)$ and $f(\rho_0, H_s)$ describe coarse features of the spectrum of H_s ; (recall Examples 2 and 3 in Sect. 2). In Theorem 3 below, we will see how the short-time control can be extended to longer times by the introduction of suitable comparison dynamics.

(vi) Equality holds in (52) if the upper and lower bound coincide, in which case the upper and lower bound simultaneously equal p_t . This is characterized in Theorem 2. But equality in (52) may also only hold in one or the other inequality, i.e., for the upper or lower bound only. Simple examples for nonsimultaneous equality are given in Table III.

Table III. Examples in which the upper or lower bound (52) reproduces the exact value of p_t . The system is a two-level system with Hamiltonian $H = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}$. The initial state and reference projection are $\rho_0 = |\psi_0\rangle\langle\psi_0|$ and $P = |\varphi\rangle\langle\varphi|$. The equality of p_t to the upper or lower bound, as stated in the last column, is restricted to $0 \leq t \leq \pi\hbar / |E_1 - E_2|$ in the first two examples, and to $0 \leq t \leq \pi\hbar / (2 |E_1 - E_2|)$ in the last two examples.

ψ_0	φ	p_t
$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\cos^2(E_1 - E_2 t / (2\hbar)) = \text{lower bound}$
$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$	$\sin^2(E_1 - E_2 t / (2\hbar)) = \text{upper bound}$
$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\frac{1}{2} (1 + \sin(E_1 - E_2 t / \hbar)) = \text{upper bound}$
$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$	$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\frac{1}{2} (1 - \sin(E_1 - E_2 t / \hbar)) = \text{lower bound}$

Thus, Table III illustrates that the bounds (52) may reproduce p_t even if p_t is nonstationary. General conditions for nonsimultaneous equality in (52) can be derived from the proof of Proposition 1, i.e., from indentifying the conditions for equality in (39a,b), using Theorem 1. We do not write down the general conditions because they involve the propagators and hence do not yield simple predictive criteria.

5. COMPARISON DYNAMICS AND VARIATIONAL PRINCIPLE

An important feature of Theorem 2 is that the orthogonal projection P can be chosen arbitrarily. In particular, it is perfectly legitimate to take for P an orthogonal projection that has a parametric dependence on t . The idea is that if one chooses the parametric dependence so as to include part of the time evolution generated by H_t (i.e., so as to approximate the Heisenberg evolution of a given projection P), one expects to be able to improve the bounds (52). The following theorem implements this idea for any ansatz for an approximate time evolution.

Theorem 3 (Time-energy uncertainty relation with comparison dynamics). The hypotheses and notation are as in Theorem 1. In addition, let a family of unitary operators W_t (trial propagators), differentiable with respect to t and satisfying $W_0 = 1$, be given.

Then p_t is bounded from above and below by

$$p_t \leq \sin^2(\arcsin \sqrt{\text{tr}(\tilde{P}_t \rho_0)} \pm \hbar^{-1} \min\{\int_0^t f(\tilde{P}_t, \tilde{H}_s) ds, \int_0^t f(\rho_0, \tilde{H}_s) ds\}) \quad (56)$$

$$\tilde{P}_t := W_t^* P W_t \quad (57)$$

$$\tilde{H}_t := W_t^* H_t W_t - i\hbar W_t^* \dot{W}_t \quad (58)$$

for all $t \geq 0$. Furthermore, one has

$$p_t = \min_W T_+(t, \rho_0, P, W.) \quad (59a)$$

$$= \max_W T_-(t, \rho_0, P, W.) \quad (59b)$$

for all $t \geq 0$, where $T_{\pm}(t, \rho_0, P, W.)$ denotes the right-hand side of (56) as a function of t, ρ, P , and the family $W.$; (the dependence on $W.$ enters through (57) and (58)). The minimum and maximum in (59) is attained when W_s equals the exact propagator for all $0 \leq s \leq t$. When $W_s = 1$, for all $0 \leq s \leq t$, eq. (56) leads back to eq. (52).

Proof. Given (i) the propagators U_t generated by the family of Hamiltonians H_t , and (ii) the orthogonal projection $\tilde{P}_t$ defined by eq. (57), we wish to find a Hamiltonian $\tilde{H}_t$ such that the propagator $\tilde{U}_t$ generated by $\tilde{H}_t$ satisfies

$$\text{tr}(P U_t \rho_0 U_t^*) = \text{tr}(\tilde{P}_t \tilde{U}_t \rho_0 \tilde{U}_t^*) \quad (60)$$

for all ρ_0 and P . The rationale is clear: The left-hand side of (60) equals p_t , and the right-hand side of (60) can be estimated by (52) with the replacement

$$\begin{aligned} H_s &\mapsto \tilde{H}_s \\ P &\mapsto \tilde{P}_t \\ p_t &\mapsto \text{tr}(\tilde{P}_t \tilde{U}_t \rho_0 \tilde{U}_t^*) \\ p_0 &\mapsto \text{tr}(\tilde{P}_t \rho_0). \end{aligned} \quad (61)$$

This yields (56) and exploits, as announced, the circumstance that the projection in Theorem 2 may be chosen t -dependent. There remains to find the Hamiltonian $\tilde{H}_t$ satisfying (60), i.e.,

$$U_t = W_t \tilde{U}_t \quad (62)$$

$$i\hbar \dot{U}_t = H_t U_t \quad (63)$$

$$i\hbar \dot{\tilde{U}}_t = \tilde{H}_t \tilde{U}_t. \quad (64)$$

Equation (62) follows from substituting (57) into (60). The other two equations are the evolution equations for the propagators U_t and $\tilde{U}_t$. Substitution of (62) and (63) gives

$$\begin{aligned} H_t W_t \tilde{U}_t &= i\hbar \dot{W}_t \tilde{U}_t + i\hbar W_t \dot{\tilde{U}}_t \\ &= i\hbar \dot{W}_t \tilde{U}_t + W_t \tilde{H}_t \tilde{U}_t, \end{aligned} \quad (65)$$

where (64) has been used in the second line. Multiplication of (65) by W_t^* from the left and by $\tilde{U}_t^*$ from the right yields formula (58) for the transformed Hamiltonian $\tilde{H}_t$. We note that $\tilde{H}_t$ is formally selfadjoint, by the unitarity of W_t . For, the latter implies that $W_t^* W_t = W_t^* W_t$. If the trial propagator equals the exact propagator, $W_t = U_t$, then

$$\tilde{H}_t = U_t^* H_t U_t - i\hbar U_t^* (i\hbar)^{-1} H_t U_t = 0 \quad (66)$$

from (58) and (63). Thus if $W_s = U_s$ for all $0 \leq s \leq t$, then $\pm$ -part in (56) vanishes, and (56) holds as an equality. This proves (59) and the statement about the attainment of the minimum and maximum. Finally, (52) is clearly a special case of (56). $\square$

Theorem 3 treats the comparison dynamics, W_t , in a way that is reminiscent of the decomposition of the time evolution in the usual interaction picture. From this viewpoint, one has the analogy

$$\begin{aligned} W_t &\leftrightarrow \text{“free” propagator,} \\ \tilde{P}_t &\leftrightarrow \text{“free” Heisenberg evolution of } P, \\ \tilde{H}_t &\leftrightarrow \text{Hamiltonian in the “interaction picture”}. \end{aligned}$$

We use quotation marks to emphasize that W_t need not come from a separation of H_t into a free Hamiltonian and an interaction part. That is, the family of trial propagators W_t is completely arbitrary. This agrees with the fact that the transformed Hamiltonian $\tilde{H}_t$ does not refer to any free or interaction part, but depends only on H_t and W_t , as described by (58). All that is needed for (56) is that $\tilde{P}_t$ and $\tilde{H}_t$ can be explicitly computed for a given W_t . The bounds (56) may then be interpreted as estimating p_t in terms of the evolution of P or ρ_0 under W_t plus a correction term involving the Hamiltonian $\tilde{H}_s$ ($0 \leq s \leq t$).

The fact that the trial-propagator W is arbitrary converts inequality (56) into a variational principle. Indeed, since W occurs only on the right-hand side of (56), one may vary W , so as to make the upper bound minimal or the lower bound maximal. When

$W.$ is varied over all one-parameter families of unitary operators the exact value of p_t is obtained [eqs. (59a,b)]. Our variational principle provides explicit error estimates: For every $W.$, it tells us how close the approximate state $\tilde{\rho}_t := W_t \rho_0 W_t^*$ is to the exact state $\rho_t = U_t \rho_0 U_t^*$ by telling us how closely the expectation values agree on every projection P . The comparison of $\tilde{\rho}_t$ and ρ_t may be written in the symmetric form

$$| \arcsin \sqrt{\text{tr}(P \tilde{\rho}_t)} - \arcsin \sqrt{\text{tr}(P \rho_t)} | \leq \hbar^{-1} \min \left\{ \int_0^t f(\tilde{P}_s, \tilde{H}_s) ds, \int_0^t f(\rho_s, \tilde{H}_s) ds \right\}, \quad (67)$$

which is equivalent to (56) and puts the error bound into full evidence. Thus, if $W.$ is a good approximation of $U.$, then $\tilde{H}_s$ will be small and the bounds (56) will bracket p_t tightly, even when t is large. Conversely, if $W.$ is a poor approximation of $U.$, then the upper and lower bound will be close to each other only for small t and rapidly approach 1 and 0 as t grows. The dependence of (56) on the cumulative energy uncertainties reflects that the bounds (56) measure the performance of the whole family $W.$, not just of a single operator W_t .

It may happen that, for given $W., P, \rho_0$, the bounds (56) coincide and thus produce the exact value p_t even if $W_s \neq U_s$, for all $0 < s \leq t$ ("perfect performance of a wrong family"). An elementary example is the trivial guess, $W_s = 1$ for $0 \leq s \leq t$, which gives the exact value p_t whenever P or ρ_0 is a constant of motion (Theorem 2). It shows that the family $W.$, which minimizes and maximizes the functionals $T_{\pm}(t, \rho_0, P, \cdot)$ need not be unique. The origin of this degeneracy is that two different families, $W.$ and $\bar{W}.$, may act identically on P or ρ_0 ,

$$W_t^* P W_t = \bar{W}_t^* P \bar{W}_t \quad (68a)$$

$$W_t \rho_0 W_t^* = \bar{W}_t \rho_0 \bar{W}_t^*, \quad (68b)$$

in which case they may perform identically in Theorem 3. Thus, one may get a good estimate of p_t from a single guess $W.$; the estimate on p_t may be good even if $W.$ is far from the exact time evolution $U.$.

The parallels to the variational principle for stationary states are striking. There one varies a trial state so as to minimize the expectation value of the Hamiltonian. Here one varies a family of trial states $\tilde{\rho}_t$ so as to minimize the right-hand side of (67). There every fixed trial state yields an upper bound for the ground-state energy. Here every fixed family of trial states yields an upper bound, eq. (67), for the difference between the trial state and the exact state.

As an illustration of our time-dependent variational principle, we use Theorem 3 to derive a simple error estimate for the case where states are pure and a family of time-dependent states, rather than a trial propagator, is used.

Corollary 1. Consider a system with a family of time-dependent Hamiltonians H_t , a solution ψ_t of the Schrödinger equation (2b), and a family of trial states $\tilde{\psi}_t$, differentiable with respect to t and satisfying $\tilde{\psi}_0 = \psi_0$. Then, for every reference state φ and all $t \geq 0$, one has the bounds

$$| \langle \varphi | \psi_t \rangle | \stackrel{\leq}{\geq} \sin_*(\arcsin | \langle \varphi | \tilde{\psi}_t \rangle | \pm \hbar^{-1} \int_0^t \| (1 - | \tilde{\psi}_s \rangle \langle \tilde{\psi}_s |) \delta(\tilde{\psi}_s) \| ds) \quad (69a)$$

and

$$1 \geq | \langle \tilde{\psi}_t | \psi_t \rangle | \geq \cos_*(\hbar^{-1} \int_0^t \| (1 - | \tilde{\psi}_s \rangle \langle \tilde{\psi}_s |) \delta(\tilde{\psi}_s) \| ds), \quad (69b)$$

where

$$\delta(\tilde{\psi}_s) := H_s \tilde{\psi}_s - i \hbar \dot{\tilde{\psi}}_s, \quad \cos_*(x) := \sqrt{1 - \sin_*^2(x)}.$$

Equality holds in (69) if and only if there exist real numbers a_s such that $\tilde{\psi}_s = e^{ia_s} \psi_s$, for all $0 \leq s \leq t$.

Proof. We write the trial states as

$$\tilde{\psi}_t = W_t \psi_0 \quad (70)$$

where W_t is a trial-propagator satisfying the hypotheses of Theorem 3. For a given trial-state family $\tilde{\psi}_t$, the propagator family W_t is not unique, of course; but this does not matter for our purposes. Furthermore, we choose $P = | \varphi \rangle \langle \varphi |$ and $\rho_0 = | \psi_0 \rangle \langle \psi_0 |$. The energy uncertainties in Theorem 3 then become

$$f^2(\tilde{P}_t, \tilde{H}_s) = \| \tilde{H}_s W_t^* \varphi \|^2 - \langle W_t^* \varphi | \tilde{H}_s W_t^* \varphi \rangle^2 \quad (71)$$

$$\begin{aligned} f^2(\rho_0, \tilde{H}_s) &= \| \tilde{H}_s \psi_0 \|^2 - \langle \psi_0 | \tilde{H}_s \psi_0 \rangle^2 \\ &= \| (1 - | \psi_0 \rangle \langle \psi_0 |) \tilde{H}_s \psi_0 \|^2 \\ &= \| W_s (1 - | \psi_0 \rangle \langle \psi_0 |) W_s^* (H_s W_s - i \hbar \dot{W}_s) \psi_0 \|^2 \\ &= \| (1 - | \tilde{\psi}_s \rangle \langle \tilde{\psi}_s |) (H_s \tilde{\psi}_s - i \hbar \dot{\tilde{\psi}}_s) \|^2 \\ &= \| (1 - | \tilde{\psi}_s \rangle \langle \tilde{\psi}_s |) \delta(\tilde{\psi}_s) \|^2 \\ &= \| \delta(\tilde{\psi}_s) \|^2 - | \langle \tilde{\psi}_s | \delta(\tilde{\psi}_s) \rangle |^2 \end{aligned} \quad (72)$$

where (54), (57), (58), (70), unitarity of W_s , and the definition of $\delta(\tilde{\psi}_s)$ have been used. Since the energy uncertainty (71) cannot be expressed in terms of the trial states, we keep only the term $f(\rho_0, \tilde{H}_s)$ in (56), at the expense of weakening the bounds. This gives the result (69a) from (72). The result (69b) follows from (69a) by choosing the reference state equal to the trial state, $\varphi = \tilde{\psi}_t$. Equality holds in (69) if and only if, for all $0 \leq s \leq t$, the vector $\delta(\tilde{\psi}_s)$ is proportional to $\tilde{\psi}_s$. A simple calculation shows that this proportionality is equivalent to the phase factor condition claimed in Corollary 1. $\square$

Discussion of Corollary 1.

(i) A trial state $\tilde{\psi}_t$ is a good approximation of the solution ψ_t of the Schrödinger equation if the remainder of $\tilde{\psi}_t$ in the Schrödinger equation is small, $\delta(\tilde{\psi}_t) \approx 0$. Corollary 1 makes this idea precise by providing explicit bounds for ψ_t in terms of $\tilde{\psi}_s$ which are manifestly tight if $\delta(\tilde{\psi}_s)$ is small ($0 \leq s \leq t$). Interestingly, the bounds require only the norm of the component of $\delta(\tilde{\psi}_s)$ orthogonal to $\tilde{\psi}_s$, $\|(1 - |\tilde{\psi}_s\rangle\langle\tilde{\psi}_s|) \delta(\tilde{\psi}_s)\|$, to be small – not the norm of $\delta(\tilde{\psi}_s)$ itself. Thus, the bounds (69) are tight whenever $\delta(\tilde{\psi}_s)$ lies almost in the subspace spanned by $\tilde{\psi}_s$.

(ii) The result (69) says that, from a given set of trial-state families, the best approximation is not necessarily the one that minimizes the remainder $\delta(\tilde{\psi}_t)$ at the endpoint t , but the one that minimizes (in the sense of the above norm) the cumulative remainder over $0 \leq s \leq t$. This agrees with the earlier remark that our variational bounds measure the performance of a one-parameter family, here $\tilde{\psi}_s$, rather than of a single element, $\tilde{\psi}_t$.

(iii) Once the best family has been identified and the integral in (69) has been evaluated, the bounds (69a) give estimates of the overlap of the exact state ψ_t and any vector φ . This provides a complete catalogue of error estimates for the location of ψ_t in $\mathcal{H}$. The error estimate for the location of ψ_t relative to $\tilde{\psi}_t$ is given by (69b). Upon introduction of a suitable phase factor e^{ia_t} , the estimate (69b) can also be put in the form

$$\begin{aligned} \|\psi_t - e^{ia_t} \tilde{\psi}_t\| &= (2 - 2 |\langle\psi_t | \tilde{\psi}_t\rangle|)^{1/2} \\ &\leq 2 \sin_* \left(\frac{1}{2} \hbar^{-1} \int_0^t \|(1 - |\tilde{\psi}_s\rangle\langle\tilde{\psi}_s|) \delta(\tilde{\psi}_s)\| ds \right). \end{aligned} \quad (73)$$

The bound (73) may be used to re-estimate the overlap of ψ_t and φ from

$$|\langle\varphi | \psi_t\rangle| \leq |\langle\varphi | \tilde{\psi}_t\rangle| \pm |\langle\varphi | \psi_t - e^{ia_t} \tilde{\psi}_t\rangle|$$

and the Schwarz inequality. But the resulting estimate for $|\langle \varphi | \psi_t \rangle|$ is weaker than (69a), as shown by (55a).

(iv) If a trial-state family comes from a known trial-propagator family, eq. (70), or if, conversely, a given trial-state family is extended to a trial-propagator family, the bounds (69a) can be improved by including the omitted term (71). This will be further discussed in Sect. 6. No such improvement is possible in (69b) because, for $\varphi = \tilde{\psi}_t$, eqs. (71) and (72) yield $f(\tilde{P}_t, \tilde{H}_s) = f(\rho_0, \tilde{H}_s)$, i.e., identical results. Thus, the bound (69b) is optimal.

(v) The occurrence of the norm $\| (1 - |\tilde{\psi}_s\rangle\langle\tilde{\psi}_s|) \delta(\tilde{\psi}_s) \|$, rather than of $\| \delta(\tilde{\psi}_s) \|$, corresponds to the fact that (69) is a variational principle for one-dimensional subspaces of $\mathcal{H}$, rather than vectors in $\mathcal{H}$. Indeed, the norm $\| (1 - |\tilde{\psi}_s\rangle\langle\tilde{\psi}_s|) \delta(\tilde{\psi}_s) \|$ is independent of the phase factor of the trial state, but $\| \delta(\tilde{\psi}_s) \|$ is not. If interpreted in terms of subspaces, the family that minimizes or maximizes the right-hand side of (69a) is unique. The nonuniqueness of the minimizing and maximizing family W in Theorem 3 disappears in Corollary 1, because when we consider a specific family of density operators $W_t \rho_0 W_t^*$, as we do in Corollary 1, the degeneracy (68) is automatically lifted.

6. COMPARISON WITH EARLIER WORK

Special cases of Theorem 2 (time-energy uncertainty relation without comparison dynamics) have been obtained previously. For a general time-independent Hamiltonian H , Fleming [29] and Bhattacharyya [30] showed that the solution ψ_t of (2b) satisfies

$$|\langle \psi_0 | \psi_t \rangle| \geq \cos_*((\langle \psi_0 | H^2 \psi_0 \rangle - \langle \psi_0 | H \psi_0 \rangle^2)^{1/2} t / \hbar). \quad (74)$$

This is the lower bound (52) and (53) for the special case $P = \rho_0 = |\psi_0\rangle\langle\psi_0|$, recalling (54) and noting that (52) and (53) coincide if the Hamiltonian is time-independent. It is also the bound (69b) for the special case where the trial family is $\tilde{\psi}_s = \psi_0$, $0 \leq s \leq t$, with remainder $\delta(\tilde{\psi}_s) = H\psi_0$. The result (74) was used in [29,30] to deduce the bound (5) for the half-life time τ_2 and the death time τ_3 of the initial state ψ_0 .

For a general family of time-dependent Hamiltonians H_t , a one-dimensional projection $P = |\varphi\rangle\langle\varphi|$, and a pure state $\rho_0 = |\psi_0\rangle\langle\psi_0|$, the bounds (52), (53), with (54), were obtained in [15], including the examples in Table III. The bounds were used to investigate revival times, the onset of the asymptotic power law (12), and various pulsed-field problems

(see also [41]). It was claimed in [15] that the bounds (53) hold without restrictions, under the condition that P and ρ_0 have rank one. But we have found a gap in the arguments for that claim. So at present, (53) is established only if the Hamiltonians at different times commute with each other. All other assertions in [15] remain unaffected.

To compare Theorem 3 with results in the literature, we first consider the variational principle implied by Theorem 3 and illustrated in Corollary 1. To the best of our knowledge, Corollary 1 is the first time-dependent variational principle with explicit error bounds for the exact state ψ_t in terms of the trial states $\tilde{\psi}_s$. All previous time-dependent variational principles for state vectors approximate ψ_t by an extremalized trial state $\tilde{\psi}_t$, without error estimates; (see [20, 42, 43] for some complementary reviews). One popular such principle, attributed to McLachlan [43, 44], minimizes the norm of the vector $\delta(\tilde{\psi}_t)$ defined in Corollary 1. It provides no error bars because, as discussed in Sect. 5, smallness of $\|\delta(\tilde{\psi}_t)\|$ gives no information about closeness of $\tilde{\psi}_t$ to ψ_t when $\|\delta(\tilde{\psi}_t)\| > 0$. Thus, Corollary 1 may be viewed as supplying the error bounds missing in McLachlan's variational principle, and improving the principle through the replacement of the norm $\|\delta(\tilde{\psi}_s)\|$ by the norm $\|(1 - |\tilde{\psi}_s\rangle\langle\tilde{\psi}_s|)\delta(\tilde{\psi}_s)\|$.

At the level of trial propagators, however, Theorem 3 is not the first time-dependent variational principle. Spruch [16] derived upper and lower bounds for the overlap of the solution ψ_t of (2b) and any reference state φ that amount to

$$|\langle\varphi|\psi_t\rangle| \lesseqgtr |\langle\varphi|W_t\psi_0\rangle| \pm \hbar^{-1} \int_0^t \|(H_s W_s - i\hbar \dot{W}_s) W_t^* \varphi\| ds, \quad (75)$$

for a trial-propagator family W as in Theorem 3. Spruch's bounds, (75), can be recovered from Theorem 3 as follows: If we choose $P = |\varphi\rangle\langle\varphi|$, $\rho_0 = |\psi_0\rangle\langle\psi_0|$, and keep only the term $f(\tilde{P}_t, \tilde{H}_s)$ in (56), we obtain

$$\begin{aligned} |\langle\varphi|\psi_t\rangle| &\lesseqgtr \sin_*(\arcsin |\langle\varphi|W_t\psi_0\rangle| \pm \hbar^{-1} \int_0^t f(\tilde{P}_t, \tilde{H}_s) ds) \\ &\lesseqgtr |\langle\varphi|W_t\psi_0\rangle| \pm \hbar^{-1} \int_0^t f(\tilde{P}_t, \tilde{H}_s) ds \\ &\lesseqgtr |\langle\varphi|W_t\psi_0\rangle| \pm \hbar^{-1} \int_0^t \|\tilde{H}_s W_t^* \varphi\| ds. \end{aligned} \quad (76)$$

In the second line, we have used the inequality (55b); and in the third line, we have inserted (71), dropping the second term in (71). By (58) and unitarity of W_s , the third line is the same as (75).

This derivation of (75) from (56) shows that Theorem 3 strengthens and extends Spruch's bounds. It puts into evidence the complementary nature of Spruch's bounds and the bounds in Corollary 1, one originating from the energy uncertainty in the reference subspace, the other one from the energy uncertainty in the initial state. For initial-value problems, Corollary 1 is easier to apply and yields stronger results in a well-defined sense; but for final-value problems, the situation is just reversed.

For completeness' sake, we mention that Spruch [16] and Shakeshaft and Spruch [45] derived additional bounds which, in the notation of (76), read

$$| \langle \varphi | \psi_t \rangle | \leq | \langle \varphi | W_t (1 - \hbar^{-1} \int_0^t \tilde{H}_s ds) \psi_0 \rangle | \pm \hbar^{-2} \int_0^t \| \tilde{H}_s \psi_0 \| \int_s^t \| \tilde{H}_{s'} W_{t'}^* \varphi \| ds' ds. \quad (77)$$

In these bounds, the initial state is propagated by a non-unitary operator, $W_t(1 - i\hbar^{-1} \int_0^t \tilde{H}_s ds)$. Hence they are not easily compared with the results in Theorem 3, in which the initial state or reference subspace is propagated unitarily.

Our final remark concerns the connection with time-dependent perturbation theory. Clearly, the bounds (76) and (77) are perturbation-theoretic in nature (see also [16, 45]); and so is Theorem 3. Indeed, returning to our analysis, one finds that in Theorem 3 we have used nothing more than a variant of second-order, time-dependent perturbation theory (Dyson series for $U_t W_t^*$ to first order). The efficiency of our method depends entirely on our ability to construct a comparison dynamics W_t approximating U_t with sufficient precision on a *subspace* of the Hilbert space of state vectors (before applying time-dependent perturbation theory). The subspace is either the range of P or the range of ρ_0 . A similar comparison dynamics is required in [16, 45], except that there the subspace is one-dimensional.

Our methods are reminiscent of Nekhoroshev's perturbation theory in classical mechanics [17]. For example, our applications in the next section will lead to exponentially long time scales analogous to the exponential time scales governing the energy exchange between constrained ("frozen") and unconstrained classical degrees of freedom, obtained by Nekhoroshev-type methods [46, 47], although our systems will be very different from those studied in [46, 47]. Actually, all results proven in Sects. 3-5 have a straightforward translation into results concerning classical dynamical systems with flows generated by volume-preserving vector fields, in particular Hamiltonian systems. In this translation, one describes states by probability measures on phase space; a projection operator is the

characteristic function of a subset of phase space; H is the Liouville operator; and good comparison dynamics may be obtained by applying, for example, the Nekhoroshev method.

7. EXAMPLES AND EXTENSIONS

A variety of applications of Theorem 2 (time-energy uncertainty relation without comparison dynamics), specialized to pure states and one-dimensional projections P , have been presented in Ref. [15]. In this section, we sketch applications of Theorem 3 to problems that involve mixed states and higher-dimensional projections. Specifically, we want to explore the quality of the bounds (56) for carefully chosen comparison dynamics.

Application 1 (Quantum-mechanical particle in a potential well).

We study the dynamics of a quantum-mechanical particle moving in $\mathbb{R}^n$ under the influence of a volcano-shaped potential v_θ , with

$$v_\theta(\underline{x}) := \theta^2 v\left(\frac{\underline{x}}{\theta}\right), \quad 1 \leq \theta < \infty, \quad (78)$$

where $v(\underline{x})$ is a smooth function on $\mathbb{R}^n$ with the following properties:

- (i) The origin $\underline{x} = 0$ is a local minimum of v , with $v(0) = 0$.
- (ii) The hessian of v at $\underline{x} = 0$ is positive-definite, with eigenvalues $\Omega_i^2 > 0$, $i = 1, \dots, n$.
- (iii) Let $g(\underline{x})$ be a smooth function, with $g(\underline{x}) = 1$, for $|\underline{x}| \leq \frac{1}{2}$, and $g(\underline{x}) = 0$, for $|\underline{x}| \geq 1$.

We define $g_{\epsilon, \theta}$ by

$$g_{\epsilon, \theta}(\underline{x}) := g\left(\frac{\underline{x}}{(\epsilon\theta)^{1/3}}\right), \quad \epsilon > 0. \quad (79)$$

Let us choose coordinates, $x_1, \dots, x_n$, on $\mathbb{R}^n$ in which the hessian of v at $\underline{x} = 0$ is diagonal. In accordance with the assumed smoothness of v , we may require that

$$\max_{\underline{x}} g_{\epsilon, \theta}(\underline{x}) \left| v_\theta(\underline{x}) - \frac{1}{2} \sum_{i=1}^n \Omega_i^2 x_i^2 \right| \leq c_1 \epsilon, \quad (80)$$

for some constant c_1 and any $\epsilon > 0$.

- (iv) Finally we assume that $|v(\underline{x})|$ is polynomially bounded.

A typical function v with these properties is sketched in *Fig. 1*, below. We note that v_θ is a potential well of diameter $O(\theta)$, with walls of height $O(\theta^2)$ and of width $O(\theta)$.

Fig. 1

The Hilbert space of the system is given by

$$\mathcal{H} = L^2(\mathbb{R}^n, d^n x), \quad (81)$$

and the Hamiltonian is

$$H \equiv H_\theta := \frac{\hbar^2}{2m} \Delta + v_\theta(\underline{x}), \quad (82)$$

where m is the mass of the particle and $\theta < \infty$. We are interested in estimating the life time of a state which, at time $t = 0$, is localized well inside the well of the volcano, asymptotically when θ becomes large. In order to derive precise estimates on such life times, we consider a comparison dynamics generated by the Hamiltonian

$$H_1 \equiv H_{1,\theta} := H_0 + w_{\varepsilon,\theta}(\underline{x}), \quad (83)$$

where

$$H_0 = -\frac{\hbar^2}{2m} \Delta + \frac{1}{2} \left(\sum_{i=1}^n \Omega_i^2 x_i^2 \right),$$

and

(84)

$$w_{\varepsilon, \theta}(\underline{x}) = g_{\varepsilon, \theta}(\underline{x}) \left[v_{\theta}(\underline{x}) - \frac{1}{2} \left(\sum_{i=1}^n \Omega_i^2 x_i^2 \right) \right].$$

In order to simplify our notations, we choose units in which $\hbar = m = 1$.

We start by considering the harmonic oscillator Hamiltonian H_0 defined in (84). With the units and conventions just fixed, the spectrum of H_0 consists of the eigenvalues

$$E_{\underline{\ell}} = \sum_{i=1}^n \Omega_i \left(\ell_i + \frac{1}{2} \right), \quad (85)$$

where $\underline{\ell} = (\ell_1, \dots, \ell_n)$, and $\ell_i = 0, 1, 2, \dots$, for $i = 1, \dots, n$, corresponding to the eigenfunctions

$$\psi_{\underline{\ell}}(\underline{x}) = \prod_{i=1}^n \Omega_i^{1/4} h_{\ell_i}(\sqrt{\Omega_i} x_i), \quad (86)$$

and h_{ℓ} is the usual ℓ^{th} Hermite function normalized such that $\int dx h_{\ell}(x)^2 = 1$. The properties of the functions h_{ℓ} are well known; in particular,

$$|h_{\ell}(x)| \leq c_{\ell, \delta} \exp \left(- \left(\frac{1}{2} - \delta \right) x^2 \right), \quad (87)$$

where, for any $\ell < \infty$ and $\delta > 0$, $c_{\ell, \delta}$ is a finite constant. Given any $E < \infty$, there are finitely many sequences, $\underline{\ell}^{(1)}, \dots, \underline{\ell}^{(k_E)}$, such that

$$E_{\underline{\ell}^{(j)}} < E, \quad \text{for all } j = 1, \dots, k_E, \quad (88)$$

with $k_E \leq a_n \left(\frac{E}{\Omega_0} \right)^n$, where $\Omega_0 = \min_i \Omega_i > 0$, and a_n is a geometrical constant. Defining $|\underline{\ell}| := \max_i \ell_i$, we also have that $|\underline{\ell}^{(j)}| < \Omega_0^{-1} E$, for all $j = 1, \dots, k_E$.

We may view the Hamiltonian H_1 as a perturbation of H_0 by the potential $W_{\varepsilon, \theta}(\underline{x})$. By (80) and (84), the operator norm, $\|w_{\varepsilon, \theta}\|$, of $W_{\varepsilon, \theta}$ is bounded by $c_1 \varepsilon$, and hence we can apply analytic perturbation theory [48]. We choose a contour γ_E in the complex plane surrounding $\text{spec } H_0 \cap [0, E)$ such that

$$\text{dist}(\gamma_E, \text{spec } H_0) \equiv d_E = \frac{1}{2} \left(E_{\underline{\ell}^{(k_E+1)}} - E_{\underline{\ell}^{(k_E)}} \right) > 0. \quad (89)$$

We choose ε so small that

$$c_1 \varepsilon \leq \frac{d_E^2}{3(E + \Omega_0)}. \quad (90)$$

Then the operator

$$P_{\theta,E} = \frac{1}{2\pi i} \oint_{\gamma_E} dz (z - H_1)^{-1} \quad (91)$$

is a spectral projection of H_1 , with

$$\text{tr}(P_{\theta,E}) = k_E, \quad \text{and } \|P_{\theta,E} - P_E^0\| < 1, \quad (92)$$

where P_E^0 is the spectral projection of H_0 onto the subspace, $\mathcal{H}_E$, spanned by the eigenfunctions $\{\psi_{\underline{\ell}^{(1)}}, \dots, \psi_{\underline{\ell}^{(k_E)}}\}$.

We claim that if ψ is in the range of $P_{\theta,E}$ then there is a finite constant $C_E > 1$ such that

$$\|e^{\alpha|\underline{x}|^2} \psi\| \leq C_E \|\psi\|, \quad (93)$$

provided $\alpha > 0$ is sufficiently small (depending on ε and C_E). This follows from a Combes-Thomas argument, [49]: First, we note that, by (92), there is a vector $\varphi \in \mathcal{H}_E$ such that $\psi = P_{\theta,E}\varphi$, with $\|\varphi\| \leq \text{const.} \|\psi\|$. Using (91), we have that

$$e^{\alpha|\underline{x}|^2} \psi = \frac{1}{2\pi i} \oint_{\gamma_E} dz \{e^{\alpha|\underline{x}|^2} (z - H_1)^{-1} e^{-\alpha|\underline{x}|^2}\} e^{\alpha|\underline{x}|^2} \varphi. \quad (94)$$

By (86) - (88),

$$\|e^{\alpha|\underline{x}|^2} \varphi\| \leq \text{const.} \|\varphi\|,$$

if $\alpha < (\frac{1}{2} - \delta)\Omega_0$. Furthermore

$$e^{\alpha|\underline{x}|^2} (z - H_1)^{-1} e^{-\alpha|\underline{x}|^2} = (z - \tilde{H}_1(\alpha))^{-1},$$

where

$$\tilde{H}_1(\alpha) = H_1 + 2\alpha n - 4\alpha^2 |\underline{x}|^2 + 4\alpha \underline{x} \cdot \underline{\nabla}.$$

Choosing α small enough, we can use elementary analytic perturbation theory [48] to prove a uniform bound on

$$\|e^{\alpha|\underline{x}|^2} (z - H_1)^{-1} e^{-\alpha|\underline{x}|^2}\| = \|(z - \tilde{H}_1(\alpha))^{-1}\|,$$

for all $z \in \gamma_E$. From this and (94) the bound (93) follows by standard arguments.

Finally, we note that

$$H - H_1 =: \delta v_{\varepsilon,\theta}, \quad (95)$$

where

$$\delta v_{\varepsilon, \theta} = (1 - g_{\varepsilon, \theta}) \left[v_{\theta} - \frac{1}{2} \sum \Omega_i^2 x_i^2 \right].$$

By the definition of $g_{\varepsilon, \theta}$, the support of $\delta v_{\varepsilon, \theta}$ is outside a ball of radius $\frac{1}{2}(\varepsilon\theta)^{1/3}$. Moreover, by assumption (iv),

$$|\delta v_{\varepsilon\theta}(\underline{x})| \leq \begin{cases} 0, & |\underline{x}| \leq \frac{1}{2}(\varepsilon\theta)^{1/3}, \\ a\theta^2 + b|\underline{x}|^2 + \frac{P(\underline{x})}{\theta}, & |\underline{x}| > \frac{1}{2}(\varepsilon\theta)^{1/3}, \end{cases} \quad (96)$$

for some finite constants a and b and some polynomial $P(\underline{x})$.

With these preliminaries out of our way, we are ready to apply the bounds (56) on the probabilities p_t (see Theorem 3) to the present system. The system is an initial state described by a density matrix ρ_0 . Given some number σ , $0 < \sigma < 1$, there then exists an energy $E_{\sigma} < \infty$ such that

$$\text{tr}(\rho_0 P_{\theta, E}) \geq (1 - \sigma)^2, \quad (97)$$

for all $E \geq E_{\sigma}$ and all $\theta \geq 1$. This follows easily from the definition (91) of the projection $P_{\theta, E}$, eqs. (83) and (86) and assumption (iii), (eq. (80)).

We now set

$$\begin{aligned} U_t &= e^{-itH}, \quad W_t = e^{-itH_1}, \\ \tilde{P}_t &= W_t^* P_{\theta, E} W_t = P_{\theta, E}, \end{aligned} \quad (98)$$

where the last equation follows from the fact that $P_{\theta, E}$ is a spectral projection of $H_1 \equiv H_{1, \theta}$, (as defined in eq. (83)). We then have (see (58)) that

$$\begin{aligned} \tilde{H}_t &= W_t^* H W_t - i W_t^* \dot{W}_t \\ &= W_t^* \delta v_{\varepsilon, \theta} W_t, \end{aligned} \quad (99)$$

by (98) and (95).

Using (33b), (98) and (99), we find that

$$\begin{aligned} f(\tilde{P}_t, \tilde{H}_s) &= f(W_{t-s}^* P_{\theta, E} W_{t-s}, \delta v_{\varepsilon, \theta}) \\ &= f(P_{\theta, E}, \delta v_{\varepsilon, \theta}), \end{aligned} \quad (100)$$

where $f(R, A)$ has been defined in (23).

Eq. (28b) (Table II) says that

$$f^2(P_{\theta,E}, \delta v_{\epsilon,\theta}) = \frac{1}{2} \text{tr}(-[P_{\theta,E}, \delta v_{\epsilon,\theta}]^2).$$

We may represent $P_{\theta,E}$ as an integral operator on $\mathcal{H}$, with integral kernel denoted by $\Pi_{\theta,E}(\underline{x}, \underline{y})$. By (92) and (93), we have that

$$\int |\Pi_{\theta,E}(\underline{x}, \underline{y})|^2 e^{2\alpha(|\underline{x}|^2 + |\underline{y}|^2)} d^n x d^n y \leq (k_E C_E^2)^2, \quad (101)$$

with C_E and α as specified in (93), and k_E as in (88). Furthermore,

$$\begin{aligned} \text{tr}(-[P_{\theta,E}, \delta v_{\epsilon,\theta}]^2) &= \int |\Pi_{\theta,E}(\underline{x}, \underline{y})|^2 \times \\ &\times (\delta v_{\epsilon,\theta}(\underline{x}) - \delta v_{\epsilon,\theta}(\underline{y}))^2 d^n x d^n y. \end{aligned} \quad (102)$$

Recalling inequality (96) and using (101), we conclude that

$$0 \leq \text{tr}(-[P_{\theta,E}, \delta v_{\epsilon,\theta}]^2) \leq 2\delta_E^2 e^{-2\mu_E \theta^{2/3}}, \quad (103)$$

for some finite constants δ_E and $2\mu_E$ that depend on E . (Here $\mu_E \propto \alpha \epsilon^{2/3}$, and, by (93) and (90), α and ϵ depend on E .)

With

$$\rho_t := U_t \rho_0 U_t^* \quad \text{and} \quad p_t := \text{tr}(\rho_t P_{\theta,E}), \quad (104)$$

inequality (56) of Theorem 3, combined with inequality (97), eq. (100) and inequality (103), yields the bounds

$$p_t \stackrel{\leq}{\geq} \sin_*^2(\arcsin(1 - \sigma) \pm \int_0^t f(\tilde{P}_s, \tilde{H}_s) ds),$$

where

$$\begin{aligned} 0 \leq f(\tilde{P}_t, \tilde{H}_s) &= \sqrt{\frac{1}{2} \text{tr}(-[P_{\theta,E}, \delta v_{\theta}]^2)} \\ &\leq \delta_E e^{-\mu_E \theta^{2/3}}, \end{aligned} \quad (105)$$

for $E \geq E_\sigma$. For σ small enough,

$$\frac{\pi}{2} - \sqrt{2\sigma} \leq \arcsin(1 - \sigma) \leq \frac{\pi}{2} - \sqrt{\frac{\sigma}{2}},$$

and we find that

$$p_t \leq \sin_*^2 \left(\frac{\pi}{2} - \sqrt{2\pi} \sigma \pm t \delta_E e^{-\mu_E \theta^{2/3}} \right), \quad (106)$$

for σ small enough and $E \geq E_\sigma$. These bounds imply that the state ρ_t of the system remains in the range of the spectral projection $P_{\theta,E}$ of the operator $H_{1,\theta}$ (defined in (83)), for E large enough, with positive probability p_t (estimated by (106)), for all times t , with

$$|t| < \text{const.} e^{\mu_E \theta^{2/3}}. \quad (107)$$

This is the key result for the present example. It has the following corollary: Let Q_R be the projection onto the subspace of wave functions in $\mathcal{H}$ with support in the ball of radius R centered at the origin in $\mathbb{R}^n$. Given $E < \infty$ and $\beta > 0$, there exists a radius $R_{E,\beta} < \infty$ such that

$$\| (1 - Q_R) P_{\theta,E} \| \leq \beta, \quad (108)$$

for all $R > R_{E,\beta}$. This is an easy consequence of inequality (101). From (108) one obtains that

$$\begin{aligned} p_t &= \text{tr}(P_{\theta,E} \rho_t) = \text{tr}(Q_R P_{\theta,E} \rho_t) + \text{tr}((1 - Q_R) P_{\theta,E} \rho_t) \\ &\leq \text{tr}(Q_R P_{\theta,E} \rho_t) + \beta \\ &= q_t + \text{tr}(Q_R (P_{\theta,E} - 1) \rho_t) + \beta \\ &\leq q_t + \sqrt{q_t} \sqrt{1 - p_t} + \beta, \end{aligned} \quad (109)$$

where, in the first inequality we have used (108), we have defined q_t by

$$q_t := \text{tr}(\rho_t Q_R), \quad (110)$$

and in the last inequality we have used the cyclicity of the trace and the Schwarz inequality for the trace and have noted that $\text{tr}((P_{\theta,E} - 1)^2 \rho_t) = \text{tr}((1 - P_{\theta,E}) \rho_t) = 1 - p_t$. From (106), (109) and (108) we conclude that, for R large enough ($R > R_{E,\beta}$, $E \geq E_\sigma$, β and σ small enough),

$$q_t \geq \frac{1}{2}, \quad \text{for all } t \text{ with } |t| < \text{const.} e^{\tilde{\mu}_R \theta^{2/3}}, \quad (111)$$

for some $\tilde{\mu}_R > 0$. This means that, with high probability, a particle prepared, at time $t = 0$, in a state localized well within a “volcano” of diameter $O(\theta)$, with walls of height

$O(\theta^2)$ and width $O(\theta)$ (as described by the potential v_θ), does not escape from it, with high probability, for all times t , with

$$|t| < \exp[\text{const. } \theta^{2/3}].$$

Remarks.

(1) Let us suppose that the function v is C^4 and has vanishing third derivatives at its local minimum $\underline{x} = 0$; (this has not been assumed in the analysis presented above, see (80)). In this case, we redefine the function $g_{\varepsilon, \theta}(\underline{x})$ (see (79)) by setting

$$g_{\varepsilon, \theta}(\underline{x}) := g\left(\frac{\underline{x}}{\sqrt{\varepsilon\theta}}\right), \quad (112)$$

with ε small enough. Under the present hypotheses, inequality (80) holds for the function $g_{\varepsilon, \theta}$ defined in (112). Going through our analysis, step by step, we then find that inequality (103) can be improved to

$$0 \leq \text{tr}(-[P_{\theta, E}, \delta v_\theta]^2) \leq 2\delta_E^2 e^{-2\mu_E \theta}, \quad (103')$$

and (111) turns out to hold for all times t , with

$$|t| \leq \exp[\text{const. } \theta], \quad (113)$$

i.e., for exponentially large times.

One may wonder whether (113) can be improved, under suitable assumptions on v , to superexponentially large times. Actually, it is easy to see that if $v(\underline{x}) \rightarrow \text{const.}$, as $|\underline{x}| \rightarrow \infty$, (i.e., the “volcano” does not permanently confine the particle) (113) cannot be improved without changing the comparison dynamics. This is seen by carefully retracing the steps of our analysis. In order to improve on (113), one would have to use a comparison dynamics involving a potential that grows faster than $|\underline{x}|^2$, as $|\underline{x}| \rightarrow \infty$. Examples of functions v for which this idea can be implemented can be constructed without difficulty.

(2) There is another, perhaps more natural (but analytically somewhat more subtle) way of rescaling the function v to a potential v_θ : One sets

$$v_\theta(\underline{x}) = \theta^2 v(\underline{x}).$$

We suppose that v satisfies assumptions (i), with $v(0) = 0$ (without loss of generality), and (ii); but (iii) is replaced by the following condition: Let g be as in (iii), but we define

$$g_\varepsilon(\underline{x}) := g\left(\frac{\underline{x}}{\varepsilon}\right)$$

and set

$$w_{\varepsilon,\theta}(\underline{x}) := g_\varepsilon(\underline{x}) \left[v_\theta(\underline{x}) - \frac{\theta^2}{2} \left(\sum_{i=1}^n \Omega_i^2 x_i^2 \right) \right].$$

We assume that

$$(iii') \quad |w_{\varepsilon,\theta}(\underline{x})| \leq \lambda(\varepsilon) \frac{\theta^2}{2} \left(\sum_{i=1}^n \Omega_i^2 x_i^2 \right),$$

for all $\underline{x} \in \mathbb{R}^n$, where $\lambda(\varepsilon) \rightarrow 0$, as $\varepsilon \rightarrow 0$.

We keep property (iv) of v as above. We then define

$$\begin{aligned} H_0 &:= -\frac{\hbar^2}{2m} \Delta + \frac{\theta^2}{2} \left(\sum_{i=1}^n \Omega_i^2 x_i^2 \right) \\ H_1 &:= H_0 + w_{\varepsilon,\theta} \end{aligned}$$

and then

$$H = H_1 + \delta v_{\varepsilon,\theta},$$

where

$$\delta v_{\varepsilon,\theta}(\underline{x}) := (1 - g_\varepsilon(\underline{x})) \left[v_\theta(\underline{x}) - \frac{\theta^2}{2} \left(\sum_{i=1}^n \Omega_i^2 x_i^2 \right) \right].$$

Then the spectrum of H_0 consists of the eigenvalues

$$E_{\underline{\ell}} = \sum_{i=1}^n \theta \Omega_i \left(\ell_i + \frac{1}{2} \right), \quad \ell_i = 0, 1, 2, \dots, \quad i = 1, \dots, n,$$

corresponding to the eigenfunctions

$$\psi_{\underline{\ell}}(\underline{x}) = \prod_{i=1}^n (\theta \Omega_i)^{1/4} h_{\ell_i}(\sqrt{\theta \Omega_i} x_i)$$

which decay like $\exp(-\theta \Omega_0 |\underline{x}|^2)$, for $\Omega_0 = \min_j \Omega_j$. By assumption (iii'), we have that

$$\|w_{\varepsilon,\theta} \psi\| \leq \lambda(\varepsilon) \|H_0 \psi\|,$$

for all ψ in the domain of definition of H_0 , and hence we can apply analytic perturbation theory to determine the eigenvalues of H_1 below an energy $E = \mathcal{E}\theta$, $\mathcal{E} < \infty$, for ε sufficiently small. The Combes-Thomas argument (see (93), (94)) can be used, just as well as before, to show that the corresponding eigenfunctions of H_1 decay like $\exp[-\alpha_\mathcal{E}\theta |\underline{x}|^2]$, for some $\alpha_\mathcal{E} > 0$. Let $P_\mathcal{E}$ denote the spectral projection of H_1 onto the subspace spanned by eigenfunctions corresponding to eigenvalues $\leq \mathcal{E}\theta$. Preparing the system in a state ρ_0 with the property that

$$\text{tr}(\rho_0 P_\mathcal{E}) \geq (1 - \sigma)^2, \quad 0 \leq \sigma \ll 1,$$

one can then prove that $p_t := \text{tr}(\rho_t P_\mathcal{E})$ remains strictly positive for all times t , with

$$|t| \leq e^{\mu_\mathcal{E} \theta},$$

for some $\mu_\mathcal{E} > 0$. As in (108)-(111), this result implies that the time of escape from the interior of the volcano to the outside world of a particle prepared, at time $t = 0$, in the state ρ_0 described above is exponentially large in θ .

We refrain from presenting details of the proofs of these claims and discussing various other variants of such results which the reader will find easy to work out.

For discussion of and references to other related results see [50].

Application 2 (one-electron ion in a magnetic field)

The system we consider here consists of a single electron bound to a nucleus of charge $(Z + 1)e$ and mass $M \gg m$, where m denotes the electron mass. Physically, $M \propto Z M_p$, where M_p is the mass of a proton. At time $t = 0$, the nucleus and the electron are supposed to form a bound state; the initial state, ρ_0 , for the relative motion is supposed to be a density matrix constructed from energetically low-lying orbitals. The system is under the influence of a constant magnetic field $\vec{B} = (0, 0, B)$ in the z -direction. The initial state, χ_0 , for the center-of-mass motion is assumed to be peaked in a point $\vec{X}_0 = (r, 0, 0)$, and its Fourier transform, $\hat{\chi}_0$, to be peaked in a momentum $\vec{P}_0 = M\vec{V}_0$, where $\vec{V}_0 = (0, -r\omega_c, 0)$, and ω_c is the cyclotron angular velocity of a particle of electric charge $q = Ze$ and mass M , i.e.

$$\omega_c = \frac{qB}{Mc}. \quad (114)$$

By Heisenberg's uncertainty relations,

$$\Delta \vec{X}_0 \cdot \Delta \vec{V}_0 \geq 3 \frac{\hbar}{M}.$$

If Z is large $M \propto ZM_p$ is large, and hence the uncertainties of position, $\Delta\vec{X}_0$, and velocity, $\Delta\vec{V}_0$, can be made very small. It is then justified to treat the center-of-mass motion of the ion classically over a very long interval of time. Let $\vec{X}(t)$ denote the classical position of the center of mass at time t . Then

$$\vec{X}(t) = (r \cos(\omega_c t), -r \sin(\omega_c t), 0).$$

We set

$$\Omega := \begin{pmatrix} 0 & \omega_c & 0 \\ -\omega_c & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad (115)$$

then $\vec{X}(t) = e^{\Omega t} \vec{X}_0$. Let $\vec{x}$ be an arbitrary vector in $\mathbb{R}^3$. We introduce moving coordinates

$$\vec{y} = e^{-\Omega t} \vec{x} \quad (116)$$

and define the velocity field $\vec{V}$ by

$$\vec{V}(\vec{y}) = \frac{d}{dt} (e^{-\Omega t} \vec{x}) = -\Omega \vec{y}. \quad (117)$$

If $\vec{x} = (x_1, x_2, x_3)$ are the position operators of the electron then the Coulomb potential of the electron in the field of the nucleus is given, at time t , by

$$-\frac{(Z+1)e^2}{|\vec{x} - \vec{X}(t)|} = -\frac{(Z+1)e^2}{|\vec{y} - \vec{X}_0|} =: v_c(\vec{y}). \quad (118)$$

Thus, in moving coordinates $\vec{y}$ (given by (116)), $v_c(\vec{y})$ is time-independent. It is therefore natural to formulate the Schrödinger equation for the motion of the electron in the field of the nucleus in moving coordinates, $\vec{y}$. This has been studied in some detail in [18]. The result is as follows: Let $\vec{V} = \vec{V}(\cdot, t)$ be an arbitrary, smooth, possibly time-dependent vector field generating a volume-preserving flow, ϕ_t , on $\mathbb{R}^3$, (i.e., $\vec{\nabla} \cdot \vec{V} = 0$). Then the Schrödinger-Pauli equation in moving coordinates, $\vec{y} = \phi_{-t}(\vec{x})$, is given by

$$i\hbar \frac{\partial}{\partial t} \psi_t(\vec{y}) = H_y \psi_t(\vec{y}),$$

where ψ_t is a two-component Pauli spinor, with

$$\psi_t \in \mathcal{H} := L^2(\mathbb{R}^3, d^3y) \otimes \mathbb{C}^2, \quad (119)$$

and

$$\begin{aligned}
H_y = & \left\{ \frac{1}{2m_*} \left(\frac{\hbar}{i} \vec{\nabla} + \frac{e}{c} \vec{A} - m_* \vec{V} \right)^2 + v_c \right. \\
& \left. - \frac{e}{c} \vec{V} \cdot \vec{A} - \frac{m_*}{2} \vec{V}^2 \right\} \otimes 1_2 + \\
& + 1 \otimes \left\{ -\frac{g\mu}{\hbar} \vec{B} \cdot \vec{S} + 2\vec{\omega} \cdot \vec{S} \right\}, \tag{120}
\end{aligned}$$

where $m_* = \frac{mM}{m+M} \approx m$ is the reduced mass of the electron, $g \approx 2$ is its gyromagnetic factor, $\mu = \frac{e\hbar}{2mc}$ is the Bohr magneton, $\vec{S} = \frac{\hbar}{2} (\sigma_x, \sigma_y, \sigma_z)$ is the spin operator of the electron, and $\vec{\omega} = \frac{1}{2} \text{curl } \vec{V}$ (with $\vec{\omega} = (0, 0, \omega_c)$, ω_c as in (114), in our example) is the angular velocity of the moving coordinate frame. The first term on the R.S. of (120) is the kinetic energy operator in moving coordinates, with $m_* \vec{V}$ corresponding to the vector potential of the Coriolis force, the term $-\frac{e}{c} \vec{V} \cdot \vec{A}$ is a relativistic correction, due to the circumstance that, in moving coordinates, there is an electric field proportional to $\frac{|\vec{V}|}{c} |\vec{B}|$, $-\frac{m_*}{2} \vec{V}^2$ is the potential of the centrifugal force, $-\frac{g\mu}{\hbar} \vec{B} \cdot \vec{S}$ is the Zeeman energy of the magnetic moment of the electron spin, and $2\vec{\omega} \cdot \vec{S}$ comes from spin precession in the moving coordinate frame. All vectors on the R.S. of (120) are expressed in the basis of the moving frame. For simplicity we are neglecting spin-orbit interactions in (120) which, for large Z , are actually somewhat significant. For details concerning the derivation of (120) see [18].

Imposing the Coulomb gauge condition on $\vec{A}$, we find that, in the moving frame of the system we are studying,

$$\vec{A}(\vec{y}) = \frac{B}{2} (-y_2, y_1, 0), \tag{121}$$

and, by (115) and (117),

$$\vec{V}(\vec{y}) = \omega_c (-y_2, y_1, 0). \tag{122}$$

Let

$$B_* = B \left(1 - 2 \frac{m_*}{M} \frac{q}{e} \right),$$

and let $\vec{A}_*$ be the vector potential in the Coulomb gauge, whose curl is given by $(0, 0, B_*)$. Note that, since $\frac{m_*}{M} \ll 1$, B_* is approximately equal to B . Furthermore, approximating g by 2 and m_* by m , we find that

$$-\frac{g\mu}{\hbar} \vec{B} \cdot \vec{S} + 2\vec{\omega} \cdot \vec{S} \approx -\frac{g\mu}{\hbar} \vec{B}_* \cdot \vec{S}. \tag{123}$$

Actually, the fact that (123) is not a strict equation is significant and is the basis of Telégdi's precision experiment determining the g -factor of the electron. For our considerations, the deviation of the L.S. from the R.S. of (123) is however insignificant.

Finally,

$$\begin{aligned} & \left[-\frac{e}{c} \vec{A} \cdot \vec{V} - \frac{m_*}{2} \vec{V}^2 \right] (\vec{y}) \\ &= -\frac{(qB)^2}{2Mc^2} \left(\frac{e}{q} + \frac{m_*}{M} \right) (y_1^2 + y_2^2) \\ &\approx -\frac{eqB_*^2}{2Mc^2} (y_1^2 + y_2^2), \end{aligned} \quad (124)$$

since $\frac{m_*}{M} - \frac{m_*}{2} \vec{V}^2 \ll \frac{1}{2}$. Note that the potential of the centrifugal force, $-\frac{m_*}{2} \vec{V}^2$, is insignificant as compared to the term $-\frac{e}{c} \vec{A} \cdot \vec{V}$.

All these calculations show that

$$\begin{aligned} H_y \approx & \left\{ \frac{1}{2m_*} \left(\frac{\hbar}{i} \vec{\nabla} + \frac{e}{c} \vec{A}_* \right)^2 - \frac{eq}{|\vec{y} - \vec{X}_0|} \right. \\ & \left. - \frac{eqB_*^2}{2Mc^2} (y_1^2 + y_2^2) \right\} \otimes 1_2 \\ & - 1 \otimes \frac{g\mu}{\hbar} \vec{B}_* \cdot \vec{S}. \end{aligned} \quad (125)$$

The terms left out on the R.S. give corrections of order $E \cdot \frac{m}{M_p}$ to a typical energy $E \in \text{spec } H_y$. Consideration of the R.S. of (125) suggests to use relative coordinates

$$\vec{\xi} := \vec{y} - \vec{X}_0 = (y_1 - r, y_2, y_3). \quad (126)$$

Then

$$\begin{aligned} & -\frac{eqB_*^2}{2Mc^2} (y_1^2 + y_2^2) - \frac{eqB_*^2}{2Mc^2} r^2 \\ &= -\frac{eqB_*^2}{Mc^2} r \xi_1 - \frac{eqB_*^2}{2Mc^2} (\xi_1^2 + \xi_2^2). \end{aligned} \quad (127)$$

The Bohr radius a is many orders of magnitude smaller than r which, in a cyclotron, is macroscopically large. Thus, the second term in (127) is, for all practical purposes, negligible. The size of the first term is

$$\begin{aligned} \left| \frac{eqB_*^2}{Mc^2} r \xi_1 \right| &\sim \frac{eqB_*^2}{Mc^2} r a \\ &\ll \frac{q^2 B^2}{2Mc^2} r^2 = \frac{M}{2} (\omega_c r)^2. \end{aligned} \quad (128)$$

Thus, the atomic physics problem we are studying is that of an electron in the field of a static nucleus of charge $-(Z + 1)e$ in an external electromagnetic field $(\vec{E}_*, \vec{B}_*)$, with $\vec{B}_* = (0, 0, B_*)$ as above, and

$$\vec{E}_* = \left(\frac{qB_*^2}{Mc^2} r, 0, 0 \right) \quad (129)$$

which is a tiny electric field. This is the Zeeman-Stark problem. Note that, in our example, H_y is time-independent.

We are thus led to study the following general problem concerning tunnelling in atomic physics: Let $\mathcal{H}$ be as in (119), and let H_0 be the Hamiltonian for the relative motion of a one-electron ion in a uniformly bounded, time-independent, external magnetic field. Let $g(\cdot)$ be the function defined in assumption (iii) of Application 1, eq. (79). Let v be a piecewise continuous function on $\mathbb{R}^3$ with the following properties: We define

$$w_\theta(\vec{\xi}) := g\left(\frac{\vec{\xi}}{\theta}\right) v(\vec{\xi}), \quad (130)$$

for any $\theta > 1$. We assume that, for some constant $k < \infty$ and an arbitrary $\theta < \infty$, there exists some finite constant Λ_θ such that

$$\|w_\theta \psi\| \leq \Lambda_\theta \| (H_0 + k1) \psi \|, \quad (131)$$

for all vectors ψ in the domain of definition of H_0 . We also assume, for example, that, for $\theta \geq \theta_0$, for some finite θ_0 ,

$$\delta v_\theta(\vec{\xi}) := \left(1 - g\left(\frac{\vec{\xi}}{\theta}\right) \right) v(\vec{\xi}) \quad (132)$$

is polynomially bounded; (clearly, $W_\theta + \delta v_\theta = v$). We define

$$H = H_0 + \varepsilon v, \quad (133)$$

and

$$H_1 = H_{1,\theta} = H_0 + \varepsilon w_\theta, \quad (134)$$

for some $\theta \geq \theta_0$ to be chosen below. Then

$$H = H_1 + \delta v_\theta. \quad (135)$$

From standard texts on rigorous atomic physics (see e.g. [48],[50]) we know that the spectrum of H_0 consists of an infinity (for an attractive Coulomb potential) of eigenvalues,

$$E_0 \leq E_1 \leq E_2 \leq \dots < E_c,$$

corresponding to eigenfunctions $\psi_0, \psi_1, \psi_2, \dots$, and an absolutely continuous part $[E_c, \infty)$, with $E_c \geq -\frac{1}{2}g\mu \sup |\vec{B}(\vec{\xi})|$; (incidentally, from now on, we return to units in which $\hbar = 1$). Let $E < E_c$, and let $\mathcal{H}_E$ be the subspace of $\mathcal{H}$ spanned by all eigenfunctions $\psi_0, \psi_1, \dots, \psi_{k_E}$ corresponding to eigenvalues $E_0 \leq E_1 \leq \dots \leq E_{k_E} \leq E$. Then

$$E_{k_E+1} - E_{k_E} =: 2d_E > 0. \quad (136)$$

Defining $\tilde{\mu}_E := \sqrt{E_c - E}$, we have that, for all $j = 1, \dots, k_E$,

$$|\psi_j(\vec{\xi})| \leq c_{E,\delta} e^{-(\tilde{\mu}_E - \delta)|\vec{\xi}|}, \quad (137)$$

for any $\delta > 0$, where $c_{E,\delta}$ is a finite constant; see e.g. [50]. Thus, eigenfunctions of H_0 decay exponentially at infinity. Given $\theta < \infty$, with $\theta \geq \theta_0$, we shall choose ε so small that

$$\varepsilon \Lambda_\theta \ll \frac{d_E}{|E + k|}, \quad (138)$$

where k is the constant appearing in (131). Thanks to (131) and (138), we may then use analytic perturbation theory to study the point spectrum of H_1 , for sufficiently low energies, and the corresponding eigenfunctions. The ideas, here, are just essentially the same ones as those developed in Application 1; see eqs. (89)-(92). The projection operator P_E is defined by

$$P_E = \frac{1}{2\pi i} \oint_{\gamma_E} dz (z - H_1)^{-1}, \quad (139)$$

where the contour γ_E has been defined in Application 1; confer to (89)-(91). Furthermore, (92) remains true (*mutatis mutandis*).

It is well known that, in the present example, we can again apply the Combes-Thomas argument, in a way analogous to (93) and (94), and show that

$$\int |\Pi_E(\vec{\xi}, \vec{\eta})|^2 e^{2\alpha(|\vec{\xi}| + |\vec{\eta}|)} d^3\xi d^3\eta \leq (k_E C_E^2)^2, \quad (140)$$

for some constant C_E , provided $\alpha < \tilde{\mu}_E$ is small enough. Here $\Pi_E(\vec{\xi}, \vec{\eta})$ is the integral kernel of P_E , (as in Application 1). The bound (140) follows from (137), by the Combes-Thomas argument. Note that (140) claims exponential, rather than Gaussian (as in Application 1), decay of $|\Pi_E(\vec{\xi}, \vec{\eta})|$, as $|\vec{\xi}| + |\vec{\eta}| \rightarrow \infty$.

The remainder of this story is just as in Application 1. Thus, we suppose that the state of the system, with dynamics generated by the Hamiltonian H , at time $t = 0$ is

described by a density matrix ρ_0 with the property that, for some $\sigma < 1$, there exists some $E < E_c$ such that

$$\text{tr}(\rho_0 P_E) \geq (1 - \sigma)^2. \quad (141)$$

We set $p_t := \text{tr}(\rho_t P_E)$, $q_t := \text{tr}(\rho_t Q_R)$, where Q_R projects onto the subspace of Pauli spinors in $\mathcal{H}$ that vanish outside a sphere of radius R centered at the origin of $\mathbb{R}^3$. Again, by (140), we have that

$$\| (1 - Q_R)P_E \| \rightarrow 0, \quad \text{as } R \rightarrow \infty; \quad (142)$$

confer to (108). The estimate replacing (103) now reads:

$$0 \leq \text{tr}(-[P_E, \delta v_\theta]^2) \leq 2\delta_E^2 e^{-2\mu_E \theta}, \quad (143)$$

for $\theta \geq \theta_0$ (see (132)) and $E < E_c$, where δ_E is a finite constant, and μ_E is positive. Recalling that $H = H_0 + \varepsilon v$, we conclude that if $\varepsilon > 0$ satisfies (138), and for σ sufficiently small,

$$p_t \stackrel{\leq}{\equiv} \sin_*^2 \left(\frac{\pi}{2} - \sqrt{2\mp 1}\sigma \pm t\varepsilon\delta_E e^{-\mu_E \theta} \right). \quad (144)$$

Assuming that ρ_0 is chosen such that

$$\text{tr}(\rho_0 P_E) = 1, \quad \text{for some } E < E_c, \quad (145)$$

then one derives from (144) (with $\sigma = 0$), and (142) that, given any $\Delta > 0$, there exists some $R_\Delta < \infty$ and a constant $\tau_{E,\Delta} > 0$ such that if ε satisfies (138) then

$$q_t \geq 1 - \Delta, \quad (146)$$

for all $R \geq R_\Delta$ and $|t| \leq \varepsilon^{-1} \tau_{E,\Delta} e^{\mu_E \theta}$. Thus the escape time to infinity of the electron grows exponentially in θ , where θ can be chosen so large that $\varepsilon \Lambda_\theta \leq \text{const.}$; (see (138)).

Example 1. We set $\vec{B} = 0$ and choose

$$v(\vec{\xi}) = \xi_1, \quad (147)$$

i.e., $\varepsilon v(\vec{\xi}) = \varepsilon \xi_1$. This is the Stark problem for a constant, external electric field $\vec{E} = (-\frac{\varepsilon}{e}, 0, 0)$ in the x-direction. Setting $k = -E_0 + 1$ in (131), we then have that

$$\| w_\theta \psi \| \leq \theta \| \psi \| \leq \theta \| (H_0 + k1) \psi \|, \quad (131')$$

i.e., $\Lambda_\theta = \theta$. Hence, given $\varepsilon > 0$ and taking into account (138), we may set

$$\theta = \kappa_E \varepsilon^{-1}, \quad (148)$$

for some constant $\kappa_E > 0$. Then (144) and (146) yield

$$p_t \stackrel{\leq}{\geq} \sin_*^2 \left(\frac{\pi}{2} - \sqrt{2\mp 1} \sigma \pm t \varepsilon \gamma_E e^{-\nu_E \varepsilon^{-1}} \right), \quad (149)$$

and $q_t \geq 1 - \Delta$, for $R \geq R_\Delta$ and

$$|t| \leq \varepsilon^{-1} \tau_{E,\Delta} e^{\nu_E \varepsilon^{-1}}, \quad \text{where } \nu_E = \mu_E \kappa_E > 0.$$

Thus, the escape time of the electron to ∞ is exponentially large in $\frac{1}{\varepsilon}$!

Example 2. Let us finally return to the problem from which we originally started in Application 2, the problem of a one-electron ion in a magnetic field. From (125) and (127) we infer that if we set $\varepsilon = \frac{eqB^2}{Mc^2}$ then we may choose θ so large that

$$\varepsilon r \theta + \frac{\varepsilon}{2} \theta^2 \leq \kappa_E,$$

for some constant $\kappa_E > 0$. Thus, as long as $r \gg \frac{\kappa_E}{\varepsilon}$, θ grows like $\frac{1}{\varepsilon}$; but, asymptotically, as $\varepsilon \downarrow 0$, θ grows like $\frac{1}{\sqrt{\varepsilon}}$. Physically, ε is very small, so that the escape time of the electron to infinity is comparatively very large.

Remarks

- (1) The techniques developed in Application 2 can be generalized to yield lower bounds on life times of states of multi-electron ions in external electromagnetic fields.
- (2) The methods developed in this paper can be applied to prove lower bounds on the life times of excited states of atoms when the electrons are coupled to the quantized electromagnetic field. These bounds agree with those expected from perturbation theory, [51].
- (3) The methods developed in this paper are efficient for proving lower bounds on the life times of unstable states. They are not useful for obtaining upper bounds on life times or for deriving a detailed, temporal picture of a decay process. In [52], Hunziker has constructed methods complementary to ours, based on the technique of complex dilatations, in order to describe the decay of unstable states and obtain bounds on life times.

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