# Generalized time-energy uncertainty relations and bounds on lifetimes of resonances

Peter Pfeifer*

*Institut für Theoretische Physik, ETH-Hönggerberg, 8093 Zürich, Switzerland, and Laboratoire de Physique de la Matière Condensée, Ecole Polytechnique, 91128 Palaiseau, France*

Jürg Fröhlich

*Institut für Theoretische Physik, ETH-Hönggerberg, 8093 Zürich, Switzerland*

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 commutes 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 modeling a quantum dot, and the total time before which a $He^+$ ion moving in a uniform magnetic field loses its electron.

## CONTENTS



## I. 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 behaviors, 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 (Jaynes and Cummings, 1963), a prototype of two interacting quantum systems.[1] The model produces collapses and revivals of the atomic population inversion, dynamic generation of approximate product states (disentanglement), irreversible subdynamics, and spontaneously broken symmetries (Pfeifer, 1982, 1983; Gea-Banacloche, 1990, 1991, 1992a, 1992b; Averbukh, 1992; Buzek *et al.*, 1992).

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 (Broeckhove, Lathouwers, and van Leuven, 1986; Broeckhove and Lathouwers, 1992). They have been spurred by the development of very short and intense laser pulses ($10^{-14}$ s, $10^{18}$ W/cm$^2$) so as to provide a computational basis for the new processes driven or probed by such laser fields (Broeckhove and Lathouwers, 1992). 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 for obtaining 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 $\beta$, is equivalent to

*Permanent address: Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211.

[1]For a review of the model, see Barnett *et al.*, 1986.

estimating the low-lying eigenvalues $E_0<E_1<\cdots$ and the corresponding eigenprojections $P_0, P_1, \ldots$ of $H$, using

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

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

as $\beta \to \infty$. A beautiful numerical implementation of Eq. (1) has recently been carried out to obtain high-precision eigenvalues and eigenmodes of a fractal drum (Sapoval, Gobron, and Margolina, 1991; Sapoval and Gobron, 1993). Perhaps the most striking difference between $e^{-iHt/\hbar}$ and $e^{-\beta H}$ manifests itself in their path-integral representations (see, for example, Reed and Simon, 1975, Chap. X.11): 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 Sec. II 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. Section II serves to illustrate some of the ideas and goals we pursue in later sections.

In Secs. III through V 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), any 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 require only expectations of quadratic expressions in the Hamiltonian, describing the energy uncertainty in the initial state and 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 Sec. III in a general form (Theorem 1). Our bounds in Theorem 2 (Sec. IV) describe what happens when neither the initial state nor the projection onto the reference subspace 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. Nonsimultaneously, 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 of improving 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, Sec. V).

In Sec. VI, 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 by Pfeifer (1993). We then contrast Theorem 3 with earlier time-dependent variational principles, e.g., with Spruch's bounds (Spruch, 1969), which are sharpened and generalized in Theorem 3. Our bounds in Corollary 1 require knowledge only of a time-dependent family of states rather than of a trial propagator, a novel aspect of our methods. Finally, we draw some parallels between Theorem 3 and Nekhoroshev's method in classical mechanics (Nekhoroshev, 1977).

Two specific applications of our general results are worked out in Sec. VII, 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, for example, 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 by Fröhlich and Studer (1993). Both examples are instances of long-lived resonances (metastable states). In both examples, we derive accurate lower bounds on lifetimes. Our analysis also yields lower bounds on lifetimes of atomic bound states when an external electric field is turned on.

For systems with an unbounded Hamiltonian, the energy uncertainties in our results will be traces of products of unbounded operators. This raises mathematical questions of operator domains, cyclic permutability of operators under the trace, and of formally commuting operators to commute in the sense of spectral projections. We shall ignore all such questions in order not to obscure the simplicity of the ideas and results. In most applications, the verification of technical conditions ignored here will be straightforward.

## II. ESTIMATES ON TIME EVOLUTION FROM SPECTRAL PROPERTIES: EXAMPLES

We consider a system described by a Hilbert space $\mathscr{H}$ of pure-state vectors and a family of time-dependent Hamiltonians $H_t$. Mixed states are represented by density operators $\rho$ which are positive, trace-class operators on $\mathscr{H}$ of trace 1. A state at time $t$ is denoted by $\rho_t$ and is determined by the initial state $\rho_0$ by solving the Liouville equation

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

If the state $\rho_0$ is pure, then $\rho_t=|\psi_t\rangle\langle\psi_t|$, where $\psi_t$ solves the time-dependent Schrödinger equation

$$i\hbar\dot{\psi}_t=H_t\psi_t. \tag{2b}$$

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 $P\mathscr{H}$. Our goal in this paper is to obtain bounds for the function

$$p_t:=\mathrm{tr}(P\rho_t), \tag{3}$$

which is the probability of finding the system in a state in the subspace $P\mathscr{H}$ at time $t$. Every experimental question about the time evolution can be cast in the form of Eq. (3). For example, if we choose $\rho_t=|\psi_t\rangle\langle\psi_t|$ and $P=|\varphi\rangle\langle\varphi|$, then $p_t=|\langle\varphi|\psi_t\rangle|^2$, i.e., Eq. (3) gives the transition probability into some final state $\varphi$, 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 Eq. (3) describes the probability of finding subsystem $I$ in the subspace $P_I\mathscr{H}_I$. 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, $P\mathscr{H}$ the reference subspace, and $p_t$ the transition probability into the reference subspace.

As described in the introduction, we intend to use time-energy uncertainty relations as a shortcut replacing an exact solution of Eq. (2). This differs somewhat from the usual perspective which focuses attention on trying to find substitutes for the nonexisting ''time operator'' (see, e.g., Allcock, 1969; Pfeifer and Levine, 1983; Partovi and Blancenbecler, 1986, 1988; Kobe and Aguilera-Navarro, 1994) or to find analogs of the position-momentum uncertainty relation by other means. As a result, our time-energy uncertainty relations here include several unconventional examples, and they leave out examples outside the framework of Eq. (3), such as delay times in scattering theory (Messiah, 1965; Pfeifer and Levine, 1983; Galindo and Pascual, 1990) and traversal times through potential barriers (Hauge and Støvneng, 1989; Fertig, 1990; Yücel and Andrei, 1992). Two comprehensive reviews of time-energy uncertainty relations are those of Allcock (1969) and Gislason, Sabeli, and Wood (1985).

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 in which $p_t$ can be calculated without solving Eq. (2) is when $\rho_0$ or $P$ commutes with $H_t$ for all $t\in[0,T]$. Then

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

The proof, using, for example, the Trotter product formula for the propagator, is obvious. This example suggests that if $\rho_0$ 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 $\rho_0$ 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

$$\tau_j\varepsilon_j\geq\hbar\gamma_j, \tag{5}$$

where $\tau_j$ is one of several notions (labeled by $j$) of lifetime of the initial state, $\varepsilon_j$ is the associated energy uncertainty, and $\gamma_j$ is a constant. Equation (5) is a version of the rule that the lifetime is inversely proportional to the energy width. We wish to quote five mathematically rigorous examples of inequalities of the form of Eq. (5): They are the Mandelstam-Tamm inequality (Mandelstam and Tamm, 1945; Messiah, 1965; Galindo and Pascual, 1990) ($j=1$), two special cases of bounds obtained by Fleming (1973) and Bhattacharyya (1983) ($j=2,3$), the Gislason-Sabelli-Wood inequality (Gislason, Sabelli, and Wood, 1985) ($j=4$), and Wigner's inequality (Wigner, 1972) ($j=5$). In these examples, the lifetimes are defined, respectively, by

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

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

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

$$\tau_4:=\int_0^\infty|\langle\psi_0|\psi_t\rangle|^2dt, \tag{6d}$$

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

The energy uncertainties are given by

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

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

and the constants (all of them optimal) are

$$\gamma_1:=1/2, \tag{8a}$$

$$\gamma_2:=\pi/4, \tag{8b}$$

$$\gamma_3:=\pi/2, \tag{8c}$$

$$\gamma_4:=3\times 5^{-3/2}\pi, \tag{8d}$$

$$\gamma_5:=1/2. \tag{8e}$$

We first discuss the examples corresponding to $j=1,\ldots,4$. In each of them $\varepsilon_j$ is the usual definition of the

uncertainty (standard deviation) of an observable, here of $H$, in the state $\psi_0$. Thus each of them yields $\tau_j=\infty$ when $\psi_0$ 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

$$\varepsilon_j=\{\tfrac{1}{2}\mathrm{tr}(-[H,|\psi_0\rangle\langle\psi_0|]^2)\}^{1/2}, \tag{9}$$

for general $\psi_0$. The equivalence of (7a) and (9) is verified by a simple computation. The time $\tau_1$ 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 $\psi_t$ to change appreciably. The times $\tau_2$ and $\tau_3$ are the first half-life time and first death time of $\psi_0$, respectively. The time $\tau_4$, being the integrated survival probability of $\psi_0$, has the meaning of an average lifetime of $\psi_0$. None of these four inequalities makes any assumptions about the spectrum of $H$.

Wigner's inequality assumes that $H$ has an absolutely continuous spectrum and that an observer measuring $\varphi$ watches the system (particle) pass. The time $t_0$ which minimizes $(\cdots)^{1/2}$ in (6e) is the mean time of arrival at $\varphi$ of the particle. Thus $\tau_5$ is the spread in arrival time, i.e., the amount of time the particle spends in state $\varphi$. If $H$ is the kinetic-energy operator in $d$ dimensions, then $|\langle\varphi|\psi_t\rangle|^2\sim\mathrm{const}\times t^{-d}$, as $t\to\infty$, for generic initial conditions, in which case one has the trivial outcome $\tau_5=\infty$ in $d\leqslant 3$. However, if one searches for $\psi_0$ and $\varphi$ that minimize the product $\tau_5\varepsilon_5$, it may be possible to identify resonance states, their lifetimes, and energy widths for suitable $H$ (Wigner, 1972). The energy distribution function in Eq. (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 $\psi_0$, if subjected to an energy measurement in the interval $(E,E+dE)$, can be detected at $\varphi$. Thus $\varepsilon_5$ is the width of the energy distribution that $\psi_0$ and $\varphi$ have in common.

*Example 3*. A celebrated result which estimates (3), without solving (2), is Ruelle's theorem (Ruelle, 1969; Reed and Simon, 1979, Chap. XI.17; Hunziker and Sigal, 1994). The system has the Hilbert space $L^2(\mathbb{R}^n)$ and a time-independent Hamiltonian of the form $H=$ kinetic energy + potential. The initial state is $\rho_0=|\psi_0\rangle\langle\psi_0|$ where $\psi_0$ 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 Eq. (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

$$\lim_{r\to\infty}\ \inf_{t\geqslant 0}\ p_{r,t}=1 \tag{10a}$$

if $\psi_0$ is a bound state, and

$$\lim_{t\to\infty}(1/t)\int_0^t p_{r,t'}dt'=0 \tag{10b}$$

for arbitrary $r<\infty$ if $\psi_0$ is a continuum state. Equation (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. Equation (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 a singular continuous spectrum of $H$.

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

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

Clearly $\mu_{\psi_0}$ is a probability measure. The properties of $\mu_{\psi_0}$ invoked in Ruelle's theorem are slightly more refined than mere energy uncertainty. They concern the measure class of $\mu_{\psi_0}$, while the usual energy uncertainty, Eq. (7a), describes a crude global feature of $\mu_{\psi_0}$ (standard deviation). The results described in (10) illustrate the rule that the long-time behavior is governed by the fine structure of $\mu_{\psi_0}$, while the short-time behavior is controlled by the coarse structure of $\mu_{\psi_0}$. The results in Example 2 provide short-time control. Different notions of slow vs fast change therefore may require different properties of the measure $\mu_{\psi_0}$. But whatever the property of $\mu_{\psi_0}$ 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 need only know whether $\mu_{\psi_0}$ is atomic or nonatomic.

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

$$(1/t)\int_0^t p_{t'}dt'\geqslant\mathrm{const}\times t^{-D-\varepsilon} \tag{12}$$

for $t\to\infty$ and arbitrary $\varepsilon>0$, where $D$ is the fractal dimension (Hausdorff dimension) of the support of $\mu_{\psi_0}$ (Salem, 1950; Ketzmerick, Petschel, and Geisel, 1992; Holschneider, 1994). In Eq. (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 a discrete point spectrum and implies a decay slower than any power law (in agreement with the fact that $p_t$ is quasiperiodic in this case). It is the analog 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 an absolutely continuous spectrum.

It is interesting to compare the hypotheses in Eqs. (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 $\mathscr{H}$ 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 Eq. (3). Then $p_t$ either is nonzero on a dense open set of $t$ values or vanishes for all $t$; see, for example, Hegerfeldt

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

| Example | "Energy spread" | Determines |
|---|---|---|
| (7a) | $\min_{E_0}\left(\int_{-\infty}^{\infty}(E-E_0)^2 d\mu_{\psi_0}(E)\right)^{1/2}$ | $\varepsilon_j \quad (j=1,\ldots,4)$ |
| (7b) | $\min_{E_0}\left(\dfrac{\int_{-\infty}^{\infty}(E-E_0)^2\left\lvert\frac{d}{dE}\mu_{\varphi,\psi_0}(E)\right\rvert^2 dE}{\int_{-\infty}^{\infty}\left\lvert\frac{d}{dE}\mu_{\varphi,\psi_0}(E)\right\rvert^2 dE}\right)^{1/2}$ | $\varepsilon_5$ |
| (10) | $\mu_{\psi_0}$ atomic, or $\mu_{\psi_0}$ continuous | whether (10a) or (10b) applies |
| (12) | $\min\{\dim\Omega:\mu_{\psi_0}(\Omega)=1,\ \Omega$ closed$\}$ | $D$ |

(1994). This implies that if $\rho_0$ 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 by Buchholz and Yngvason (1994), this is not in conflict with Einstein causality.

## III. 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 Eq. (3). Since $p_t$ satisfies

$$i\hbar\dot{p}_t=\mathrm{tr}(P[H_t,\rho_t])=\mathrm{tr}(\rho_t[P,H_t]) \tag{13}$$

by Eqs. (2a) and (3), we seek bounds for expectations of the type $\mathrm{tr}(iR[A,B])$, where $R$ is a positive operator and $A,B$ are self-adjoint. 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 $(A|A)\geqslant 0$, for all operators $A,B,C$ in its domain and all $b\in\mathbb{C}$. Then

$$|(A|B)-(B|A)|^2 \leqslant 4|(A|B)|^2 \leqslant 4(A|A)(B|B). \tag{14}$$

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

$$(aA+ibB|aA+ibB)=0, \tag{15}$$

with

$$(a,b)\neq(0,0), \tag{16}$$

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

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

**Lemma 2** (Conventional uncertainty relation). Let $\rho$ be a density operator and $A,B$ self-adjoint operators. Then

$$|\mathrm{tr}(\rho[A,B])|^2 \leqslant 4\{\mathrm{tr}(\rho A^2)-\mathrm{tr}^2(\rho A)\}\times\{\mathrm{tr}(\rho B^2)-\mathrm{tr}^2(\rho B)\}. \tag{17}$$

Equality holds in Eq. (17) if and only if

$$\{a[A-\mathrm{tr}(\rho A)]+ib[B-\mathrm{tr}(\rho B)]\}\rho=0,$$

for some $a,b\in\mathbb{R}$ with $(a,b)\neq(0,0)$. The right-hand side of Eq. (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 $(A|B):=\mathrm{tr}(\rho A^*B)$ is a non-negative sesquilinear form. For self-adjoint $A,B$ and real numbers $a,b$ it satisfies

$$|\mathrm{tr}(\rho[A,B])|^2=|(A-a|B-b)-(B-b|A-a)|^2 \leqslant 4(A-a|A-a)(B-b|B-b) \tag{18}$$

by use of Eq. (14). Minimization of the bound (18) with respect to $a$ and $b$, using $\mathrm{tr}(\rho)=1$, yields Eq. (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 $\mathrm{tr}(\rho C^*C)=0$ is equivalent to $C\rho=0$ for arbitrary $C$. □

The usual application of Eq. (17) is to estimate the standard deviations $\{\cdots\}^{1/2}$ 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 $\rho$ 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 $A,B$ self-adjoint operators. Then

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 (II.1)–(II.3) are all non-negative.

| | $f^2(R,A)$ | | Bounds |
|---|---|---|---|
| $R=\rho=\|\psi\rangle\langle\psi\|$ | $=\mathrm{tr}(\rho A^2-\rho A\rho A)$ | (II.1a) | (17), (19), and (22) coincide |
| | $=\mathrm{tr}(\rho A^2)-\mathrm{tr}^2(\rho A)$ | (II.1b) | |
| | $=\langle\psi\|A^2\psi\rangle-\langle\psi\|A\psi\rangle^2$ | (II.1c) | |
| $R=\rho=\rho^*\geqslant 0$, $\mathrm{tr}(\rho)=1$ | $\leqslant\mathrm{tr}(\rho A^2)-\mathrm{tr}^2(\rho A)$ | (II.2) | (22) implies (17) |
| $R=P=P^*=P^2$ | $=\mathrm{tr}(PA^2-PAPA)$ | (II.3a) | (19) and (22) coincide |
| | $=(1/2)\mathrm{tr}(-[P,A]^2)$ | (II.3b) | |

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

Equality holds in Eq. (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

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

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

where Eq. (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 self-adjoint $A$ and $B$, it gives

$$(A|B)-(B|A)=\mathrm{tr}(PAB-PAPB-PBA+PBPA)$$
$$=\mathrm{tr}(P[A,B]). \tag{21}$$

Substitution of Eqs. (20) and (21) into (14) yields Eq. (19). Next, consider an arbitrary $C$ such that $(C|C)=0$. From Eq. (20) it follows that $\langle CP\psi|(1-P)CP\psi\rangle=0$, for all $\psi$. This implies $CP\psi\in P\mathscr{H}$ for all $\psi$, 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 self-adjoint $C$. Together with Lemma 1, this proves the conditions for equality in Eq. (19) and for zero right-hand side of (19). □

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

$$|\mathrm{tr}(R[A,B])|^2 \leqslant 4f^2(R,A)f^2(R,B), \tag{22}$$

where

$$f(R,A):=\left(\sum_{n=1}^N \lambda_n\mathrm{tr}(P_nA^2-P_nAP_nA)\right)^{1/2}. \tag{23}$$

Equality holds in Eq. (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

$$(A|B):=\sum_{n=1}^N \lambda_n\mathrm{tr}(P_nA^*(1-P_n)BP_n). \tag{24}$$

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

$$(C|C)=0\Leftrightarrow CP_n=P_nCP_n \quad (\text{all } n) \tag{25a}$$

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

$$\Rightarrow [R,C]R=0 \tag{25c}$$

$$\Rightarrow \sum_n \lambda_nP_nCP_m-\lambda_mCP_m=0 \quad (\text{all } m) \tag{25d}$$

$$\Rightarrow P_mCP_m=CP_m \quad (\text{all } m) \tag{25e}$$

$$\Rightarrow (C|C)=0. \tag{25f}$$

Equation (25a) is clear from the proof of Lemma 3 and $\lambda_n>0$, for all nonzero terms in (24). Parts (25b) and (25c) 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 $(\lambda_n-\lambda_m)P_nCP_m=0$ and hence $P_nCP_m=0$ 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 self-adjoint $C$. □

We call the quantity $f(R,A)$ the uncertainty of the observable $A$ with respect to the weight $R$. For a density operator $\rho$ and an orthogonal projection $P$, we call $f(\rho,A)$ the uncertainty of $A$ in state $\rho$ and $f(P,A)$ the uncertainty of $A$ in the subspace $P\mathscr{H}$. 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 Lemma 3. Of the statements in Table II, only (II.2) needs proof. It follows from

$$f^2(\rho,A)=\mathrm{tr}(\rho A^2)-\sum_n \lambda_n \mathrm{tr}(P_n A P_n A), \tag{26}$$

$$\begin{aligned}\mathrm{tr}^2(\rho A)&=\left(\sum_n \lambda_n \mathrm{tr}(P_n P_n A P_n)\right)^2 \\ &\leqslant\left(\sum_n \lambda_n \sqrt{\mathrm{tr}(P_n^2)\mathrm{tr}((P_n A P_n)^2)}\right)^2 \qquad (27)\\ &=\left(\sum_n \sqrt{\lambda_n \mathrm{tr}(P_n)}\sqrt{\lambda_n \mathrm{tr}((P_n A P_n)^2)}\right)^2 \\ &\leqslant\left(\sum_n \lambda_n \mathrm{tr}(P_n)\right)\left(\sum_n \lambda_n \mathrm{tr}((P_n A P_n)^2)\right) \qquad (28)\\ &=\sum_n \lambda_n \mathrm{tr}(P_n A P_n A) \qquad (29)\end{aligned}$$

where we have used the Schwarz inequality $|\mathrm{tr}(X^*Y)|\leqslant\{\mathrm{tr}(X^*X)\mathrm{tr}(Y^*Y)\}^{1/2}$ in (27), the Cauchy inequality in (28), and $\mathrm{tr}(\rho)=1$ in (29).

We now discuss Theorem 1. (i) 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

$$f(rR,aA)=r^{1/2}|a|f(R,A), \tag{30a}$$

$$f(R,U^*AU)=f(URU^*,A) \tag{30b}$$

($r\geqslant 0; a\in\mathbb{R}; U=$ unitary) ensure that both sides of Eq. (22) transform in the same way under rescaling and unitary transformation of the operators. Equation (30b) also ensures that the function $f$ is unitarily invariant, $f(U^*RU,U^*AU)=f(R,A)$, as a good measure of noncommutativity should be. For given observables $A$ and $B$, the condition

$$[R,aA+ibB]R=0, \quad a^2+b^2>0, \tag{31}$$

for some $a,b\in\mathbb{R}$ defines the class of minimum-uncertainty weights $R$, i.e., the weights for which equality holds in Eq. (22). If $A$ and $B$ are the position and momentum of a particle, and one chooses $R=|\psi\rangle\langle\psi|$, the condition (31) reduces to the familiar characterization of coherent states. Since the inequality (22) is tighter than (17), the class of weights obeying (31) 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 a pure point spectrum is a minimum-uncertainty weight.

(ii) In Sec. II, we introduced the energy uncertainty as one of several ways of measuring over how wide a part of the energy spectrum a state is spread [Eq. (7a), Table I], which suggests that $f(R,A)$, too, should reflect spectral properties of the observable $A$. The bound

$$f(R,A)\leqslant\frac{1}{2}\sqrt{\mathrm{tr}(R)}(a_+-a_-), \tag{30c}$$

in which $a_+$ and $a_-$ denote the upper and lower end of the spectrum of $A$, illustrates that this is indeed the case. It shows that the uncertainty $f(R,A)$ is limited by the width of the part of the spectrum of $A$ in the spectral support of $R$. To prove (30c), we consider an orthogonal projection $P$, choose an orthonormal basis $\{\varphi_i\}$ in $P\mathscr{H}$, and note that

$$\begin{aligned}\mathrm{tr}(PA^2-PAPA)&=\sum_i\{\langle\varphi_i|A^2\varphi_i\rangle-\langle\varphi_i|APA\varphi_i\rangle\}\\ &\leqslant\sum_i\{\langle\varphi_i|A^2\varphi_i\rangle-\langle\varphi_i|A\varphi_i\rangle^2\}\\ &=\sum_i\{(a_+-\langle\varphi_i|A\varphi_i\rangle)(\langle\varphi_i|A\varphi_i\rangle-a_-)\\ &\quad-\langle\varphi_i|(a_+-A)(A-a_-)\varphi_i\rangle\}\\ &\leqslant\sum_i(a_+-\langle\varphi_i|A\varphi_i\rangle)(\langle\varphi_i|A\varphi_i\rangle-a_-)\\ &\leqslant\sum_i\max_{a_-\leqslant x\leqslant a_+}(a_+-x)(x-a_-)\\ &=\frac{1}{4}\mathrm{tr}(P)(a_+-a_-)^2,\end{aligned}$$

using $|\varphi_i\rangle\langle\varphi_i|\leqslant P$ and $(a_+-A)(A-a_-)\geqslant 0$ in the second and fourth line, respectively. This, together with Eq. (23), proves Eq. (30c). The bound (30c) is a variant of what is known as Grüss' inequality (Mitrinović, 1970). Nontrivial examples in which the bound holds as equality are given in the next paragraph.

(iii) The unequal role of the weight $R$ and the observable $A$ in $f(R,A)$ is highlighted by the scaling property (30a) and entails $f(R,A)\neq f(A,R)$ in general. However, if $P$ and $Q$ are orthogonal projections, then

$$f(P,Q)=f(Q,P)\leqslant\frac{1}{2}\min\{\sqrt{\mathrm{tr}(P)},\sqrt{\mathrm{tr}(Q)}\}, \tag{30d}$$

where the second part is an application of Eq. (30c). Hence the uncertainty of $Q$ in the subspace $P\mathscr{H}$ is equal to the uncertainty of $P$ in the subspace $Q\mathscr{H}$ and is limited by the dimension of the smaller of the two subspaces. An interesting consequence of (30d) is that, by the one-to-one correspondence between noncommuting orthogonal projections and incompatible yes-no experiments (see, for example, Jauch, 1968), it endows the propositional calculus of quantum mechanics with a numerical measure of incompatibility, $f(P,Q)$, which preserves the symmetry of the relation "incompatible" between two propositions and identifies two propositions as maximally incompatible when the upper bound in (30d) is reached. An elementary example of maximally incompatible propositions according to this criterion are the one-dimensional eigenspaces of different spin components $S_x,S_y,S_z$ of a spin-$\frac{1}{2}$ particle. A more general example, in $\mathscr{H}=\mathbb{C}^n$, is obtained by taking $P\mathscr{H}$ as the $m$-dimensional subspace of vectors $(x_1,\ldots,x_n)$ with $x_i=0$ for $i=1,\ldots,n-m$ $(1\leqslant m\leqslant n/2)$ and $Q\mathscr{H}$ as the $[(n+1)/2]$-dimensional subspace of vectors with $x_i=x_{n-i+1}$ for $i=1,\ldots,n$. In this case, the upper bound in

Eq. (30d) is reached by virtue of $PQP=\frac{1}{2}P$, showing that the bound is optimal in all dimensions.

(iv) We close our discussion with a remark about improvements upon Theorem 1. It concerns the question whether Eq. (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 $R=\Sigma_n\lambda_n P_n$, $\lambda_n\geqslant 0$, 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

$$f^2(P',A)+f^2(P'',A)-f^2(P,A)=2\ \mathrm{tr}(P'AP''AP')\geqslant 0. \tag{32}$$

Thus Theorem 1 appears to be optimal.

## IV. 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 in which the Hamiltonian is time dependent, it is useful first to 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 $t$. This satisfies the equation

$$U_{t,s}=1-(i/\hbar)\int_s^t H_{t'}U_{t',s}dt' \tag{33}$$

for all $s$, $t\in\mathbb{R}$.[2] Let $\rho_0$ be a fixed density operator and $P$ an orthogonal projection. Define

$$\rho_{t,s}:=U_{t,s}\rho_0 U_{t,s}^* \tag{34}$$

$$p_{t,s}:=\mathrm{tr}(P\rho_{t,s}). \tag{35}$$

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

$$\left|\frac{\partial}{\partial t}p_{t,s}\right|\leqslant 2\hbar^{-1}f(P,H_t)\sqrt{p_{t,s}-p_{t,s}^2} \tag{36a}$$

$$\left|\frac{\partial}{\partial s}p_{t,s}\right|\leqslant 2\hbar^{-1}f(\rho_0,H_s)\sqrt{p_{t,s}-p_{t,s}^2} \tag{36b}$$

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

*Proof.* Equation (33) implies that the propagator satisfies $U_{s,t}=U_{t,s}^*$ and

$$i\hbar\frac{\partial}{\partial t}U_{t,s}=H_tU_{t,s},\quad U_{s,s}=1 \tag{37a}$$

$$i\hbar\frac{\partial}{\partial s}U_{t,s}=-U_{t,s}H_s,\quad U_{t,t}=1. \tag{37b}$$

Differentiation of Eq. (34) with respect to $t$ and $s$, together with Eqs. (37a) and (37b) and their adjoints, leads to

$$i\hbar\frac{\partial}{\partial t}\rho_{t,s}=[H_t,\rho_{t,s}], \tag{38a}$$

$$i\hbar\frac{\partial}{\partial s}\rho_{t,s}=-U_{t,s}[H_s,\rho_0]U_{t,s}^*. \tag{38b}$$

From Eqs. (35), (38a) and Theorem 1, it follows that

$$\begin{aligned}\hbar\left|\frac{\partial}{\partial t}p_{t,s}\right|&=|\mathrm{tr}(P[H_t,\rho_{t,s}])|\\&\leqslant 2f(P,H_t)f(P,\rho_{t,s}).\end{aligned} \tag{39}$$

For any orthogonal projection $P$ and density operator $\rho$, one has the inequality

$$\begin{aligned}f^2(P,\rho)&=\mathrm{tr}(P\rho(1-P)\rho)\\&=\mathrm{tr}((\sqrt{\rho}P\sqrt{\rho})^*\sqrt{\rho}(1-P)\sqrt{\rho})\\&\leqslant\{\mathrm{tr}((P\rho P)^2)\mathrm{tr}([(1-P)\rho(1-P)]^2)\}^{1/2}\\&\leqslant\{\mathrm{tr}^2(P\rho P)\mathrm{tr}^2((1-P)\rho(1-P))\}^{1/2}\\&=\mathrm{tr}(P\rho)-\mathrm{tr}^2(P\rho),\end{aligned} \tag{40}$$

where we have used Eq. (23) in the first line, the Schwarz inequality $|\mathrm{tr}(X^*Y)|\leqslant\{\mathrm{tr}(X^*X)\mathrm{tr}(Y^*Y)\}^{1/2}$ in the third line, and non-negativity of the eigenvalues of $P\rho P$ and $(1-P)\rho(1-P)$ in the fourth line. In the last line we have used that $\mathrm{tr}(\rho)=1$. Equality holds in Eq. (40) if $\rho$ is a pure state. Combination of Eqs. (39), (40), and (35) proves (36a).

From (35), (38b), and Theorem 1, it follows that

$$\begin{aligned}\hbar\left|\frac{\partial}{\partial s}p_{t,s}\right|&=|\mathrm{tr}(PU_{t,s}[H_s,\rho_0]U_{t,s}^*)|\\&=|\mathrm{tr}(\rho_0[H_s,U_{t,s}^*PU_{t,s}])|\\&\leqslant 2f(\rho_0,H_s)f(\rho_0,U_{t,s}^*PU_{t,s})\\&=2f(\rho_0,H_s)f(\rho_{t,s},P)\\&\leqslant 2f(\rho_0,H_s)\{\mathrm{tr}(\rho_{t,s}P)-\mathrm{tr}^2(\rho_{t,s}P)\}^{1/2}.\end{aligned} \tag{41}$$

In the last two lines of Eq. (41), we have used (30b) and (II.2) (see Table II). Inequality (41), together with (35), proves (36b). □

**Proposition 2**. If the Hamiltonians $H_t$ and $H_{t'}$ in Proposition 1 commute for all $t$ and $t'$, then the bounds (36a), (36b) are also valid with the replacements

$$f(P,H_t)\mapsto\min\{f(P,H_t),f(\rho_0,H_t)\} \tag{42a}$$

$$f(\rho_0,H_s)\mapsto\min\{f(P,H_s),f(\rho_0,H_s)\}. \tag{42b}$$

*Proof.* By rewriting the equations of motion (38a), (38b) as

$$i\hbar\frac{\partial}{\partial t}\rho_{t,s}=U_{t,s}[\tilde{H}_{t,s},\rho_0]U_{t,s}^* \tag{38a'}$$

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

TABLE III. Examples in which the upper or lower bound (50) reproduces the exact value of $p_t$. The system is a two-level system with Hamiltonian $H=\left(\begin{smallmatrix}E_1 & 0\\ 0 & E_2\end{smallmatrix}\right)$. 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.

| $\psi_0$ | $\varphi$ | $p_t$ |
|---|---|---|
| $(1/\sqrt{2})\begin{pmatrix}1\\1\end{pmatrix}$ | $(1/\sqrt{2})\begin{pmatrix}1\\1\end{pmatrix}$ | $\cos^2(\lvert E_1-E_2\rvert t/(2\hbar))=$ lower bound |
| $(1/\sqrt{2})\begin{pmatrix}1\\1\end{pmatrix}$ | $(1/\sqrt{2})\begin{pmatrix}1\\-1\end{pmatrix}$ | $\sin^2(\lvert E_1-E_2\rvert t/(2\hbar))=$ upper bound |
| $(1/\sqrt{2})\begin{pmatrix}1\\i\end{pmatrix}$ | $(1/\sqrt{2})\begin{pmatrix}1\\1\end{pmatrix}$ | $\frac{1}{2}(1+\sin(\lvert E_1-E_2\rvert t/\hbar))=$ upper bound |
| $(1/\sqrt{2})\begin{pmatrix}1\\-i\end{pmatrix}$ | $(1/\sqrt{2})\begin{pmatrix}1\\1\end{pmatrix}$ | $\frac{1}{2}(1-\sin(\lvert E_1-E_2\rvert t/\hbar))=$ lower bound |

$$i\hbar\frac{\partial}{\partial s}\rho_{t,s}=-[\tilde{H}_{s,t},\rho_{t,s}], \tag{38b$'$}$$

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

$$\begin{aligned}\hbar\left|\frac{\partial}{\partial t}p_{t,s}\right|&=|\mathrm{tr}(\rho_0[\tilde{H}_{t,s},U_{t,s}^{*}PU_{t,s}])|\\&\leq 2f(\rho_0,\tilde{H}_{t,s})f(\rho_0,U_{t,s}^{*}PU_{t,s})\\&\leq 2f(\rho_0,\tilde{H}_{t,s})\sqrt{p_{t,s}-p_{t,s}^2},\end{aligned} \tag{36a$'$}$$

$$\begin{aligned}\hbar\left|\frac{\partial}{\partial s}p_{t,s}\right|&=|\mathrm{tr}(P[\tilde{H}_{s,t},\rho_{t,s}])|\\&\leq 2f(P,\tilde{H}_{s,t})f(P,\rho_{t,s})\\&\leq 2f(P,\tilde{H}_{s,t})\sqrt{p_{t,s}-p_{t,s}^2}.\end{aligned} \tag{36b$'$}$$

They are quite useless in general, because, unlike in Proposition 1, the factors $f(\ldots,\ldots)$ 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 Eq. (36$'$) competes with (36) and yields the improvement (42). □

**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

$$p_{t,s}\ \begin{matrix}\leq\\ \geq\end{matrix}\ \sin_{*}^{2}\left(\arcsin\sqrt{\mathrm{tr}(P\rho_0)}\ \pm\hbar^{-1}\min\left\{\int_s^t f(P,H_\tau)d\tau,\int_s^t f(\rho_0,H_\sigma)d\sigma\right\}\right), \tag{43}$$

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

$$\sin_{*}(x):=\begin{cases}0 & \text{if } x\leq 0,\\ \sin x & \text{if } 0\leq x\leq\pi/2,\\ 1 & \text{if } x\geq\pi/2.\end{cases} \tag{44}$$

If $s>t$, the integration limits in (43) are interchanged.

*Proof.* From Proposition 1 we have the bounds

$$\pm\frac{\partial}{\partial\tau}p_{\tau,s}\leq 2\hbar^{-1}f(P,H_\tau)\sqrt{p_{\tau,s}-p_{\tau,s}^2} \tag{45}$$

$$\pm\frac{\partial}{\partial\sigma}p_{t,\sigma}\leq 2\hbar^{-1}f(\rho_0,H_\sigma)\sqrt{p_{t,\sigma}-p_{t,\sigma}^2}. \tag{46}$$

For $s<t$, integration of (45) by separation of variables, from $\tau=s$ to $\tau=t$, gives

$$\pm\int_{p_{s,s}}^{p_{t,s}}(p-p^2)^{-1/2}dp\leq 2\hbar^{-1}\int_s^t f(P,H_\tau)d\tau, \tag{47}$$

where the integral on the left-hand side is well defined because $0\leq p_{s,t}\leq 1$. For $s<t$, integration of (46), from $\sigma=t$ to $\sigma=s$, gives

$$\pm\int_{p_{t,t}}^{p_{t,s}}(p-p^2)^{-1/2}dp\geq 2\hbar^{-1}\int_t^s f(\rho_0,H_\sigma)d\sigma. \tag{48}$$

The sense of inequality (48) is opposite to that of (47), because, in (48), we integrate in the negative $\sigma$ direction. Since $p_{s,s}=p_{t,t}=\mathrm{tr}(P\rho_0)$, the two inequalities compete with each other and yield

$$\begin{aligned}&\pm\int_{\mathrm{tr}(P\rho_0)}^{p_{t,s}}(p-p^2)^{-1/2}dp\\&\quad=\pm 2(\arcsin\sqrt{\mathrm{tr}(P\rho_0)}-\arcsin\sqrt{p_{t,s}})\\&\quad\leq 2\hbar^{-1}\min\left\{\int_s^t f(P,H_\tau)d\tau,\int_s^t f(\rho_0,H_\sigma)d\sigma\right\}.\end{aligned} \tag{49}$$

Solving Eq. (49) for $\arcsin\sqrt{p_{t,s}}$ and applying the function $\sin_{*}^{2}$ on both sides of the inequality, one obtains the result (43) by monotonicity of $\sin_{*}$. □

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 $P\mathscr{H}$ [Eq. (36a)]. The rate of change in the backward time direction is bounded by the energy uncertainty in the initial state $\rho_0$ [Eq. (36b)]. Hence if we want to obtain an inequality that combines the two energy uncertainties, we have to consider a 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 $\tau$ integration of (45) is from left to right, but the $\sigma$ integration of (46) 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 ($t\geqslant 0$), with the understanding that the opposite case ($t\leqslant 0$) 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 $H_t$. Let $\rho_0$ be the initial state of the system, and choose an orthogonal projection $P$. Then the probability $p_t$, defined in Eq. (3), is bounded from above and below by

$$p_t \begin{matrix}\leqslant\\ \geqslant\end{matrix} \sin_*^2\Bigg(\arcsin\sqrt{p_0} \pm\hbar^{-1}\min\Bigg\{\int_0^t f(P,H_s)ds,\int_0^t f(\rho_0,H_s)ds\Bigg\}\Bigg) \tag{50}$$

for all $t\geqslant 0$. The functions $f$ and $\sin_*$ are defined in Eqs. (23) and (44). In the special case that $[H_s,H_{s'}]=0$ for all $0\leqslant s,s'\leqslant t$, one has the improvement

$$p_t \begin{matrix}\leqslant\\ \geqslant\end{matrix} \sin_*^2\Bigg(\arcsin\sqrt{p_0} \pm\hbar^{-1}\int_0^t \min\{f(P,H_s),f(\rho_0,H_s)\}ds\Bigg). \tag{51}$$

The upper and lower bound in Eq. (50) coincide if and only if either $[P,H_s]=0$ for all $0\leqslant s\leqslant t$ or $[\rho_0,H_s]=0$ for all $0\leqslant s\leqslant t$. The bounds (51) coincide if and only if, for all $0\leqslant s\leqslant t$, either $[P,H_s]=0$ or $[\rho_0,H_s]=0$.

*Proof.* Inequality (50) is Proposition 3, specialized to zero initial time and positive final time. Inequality (51) follows from Proposition 2: One substitutes (42a) into (36a) 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. □

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

(i) The bounds (50) 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 a finite matrix, the calculation of $f(P,H_s)$ requires three matrix multiplications [recall Eq. (II.3)]. This is clearly much less effort than to diagonalize $H_s$, as a step towards solving (2). 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 Eq. (50), estimate them by using Eq. (30c), or estimate $f(\rho_0,H_s)$ by using Eq. (II.2) (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 $\rho_0$ have infinite rank (large reference subspace or highly mixed state). In the other extreme, where $P$ and $\rho_0$ have rank one, i.e., where $P=|\varphi\rangle\langle\varphi|$ and $\rho_0=|\psi_0\rangle\langle\psi_0|$, one has

$$f(P,H_s)=(\langle\varphi|H_s^2\varphi\rangle-\langle\varphi|H_s\varphi\rangle^2)^{1/2} \tag{52a}$$

$$f(\rho_0,H_s)=(\langle\psi_0|H_s^2\psi_0\rangle-\langle\psi_0|H_s\psi_0\rangle^2)^{1/2} \tag{52b}$$

by Eq. (II.1). In this case, the energy uncertainties are the usual standard deviations with respect to vector states and simple to estimate.

(ii) The bounds (50) express a time-energy uncertainty relation, because they manifestly imply that $p_t$ remains close to its initial value $p_0$ ("large lifetime of $\rho_0$") if the energy uncertainty in $P\mathscr{H}$ or $\rho_0$ is small. Conversely, they imply that the energy uncertainty in $P\mathscr{H}$ and the energy uncertainty in $\rho_0$ must be large if $p_t$ departs rapidly from $p_0$ ("short lifetime of $\rho_0$").

(iii) By the property that $f(R,H_s)=0$ if and only if $[R,H_s]=0$, the bounds (50) clearly relate the change of $p_t$ to the degree of noncommutativity of the pairs $(P,H_s)$ and $(\rho_0,H_s)$. They show that $p_t\equiv p_0$ if $P$ or $\rho_0$ is a constant of motion. They generally show what happens if $P$ and $\rho_0$ are close to constants of motion.

(iv) The bounds (50) are invariant with respect to the interchange of $P$ and $1-P$. That is, if we write $p_t=\mathrm{tr}\,(P\rho_t)$ and $p_t'=\mathrm{tr}\,((1-P)\rho_t)$, 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 $P\mathscr{H}$ and $(1-P)\mathscr{H}$ and the associated probability interpretations of $p_t$ and $1-p_t$. Variants of the bounds (50) are obtained by applying the inequalities

$$\sin_*(\arcsin\sqrt{p_0}\pm x) \begin{matrix}\leqslant\\ \geqslant\end{matrix} \sqrt{p_0}+2\ \min\{\sqrt{1-p_0},\pm 1\}\sin_*(x/2) \tag{53a}$$

$$\begin{matrix}\leqslant\\ \geqslant\end{matrix} \sqrt{p_0}\pm x, \tag{53b}$$

for $x\geqslant 0$. We use Eqs. (53a) and (53b) in Secs. V and VI.

(v) The bounds (50) depend on the energy uncertainties in $P\mathscr{H}$ and $\rho_0$, 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 (50) 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 Sec. II). In Theorem 3 below, we shall see how the short-time control can be extended to longer times by the introduction of suitable comparison dynamics.

(vi) Equality holds in (50) if the upper and lower bounds coincide, in which case the bounds simultaneously equal $p_t$. This is characterized in Theorem 2. But equality in (50) may also hold in only one or the other inequality, i.e., for the upper or lower bound only. Simple examples for nonsimultaneous equality are given in Table III. Thus Table III illustrates that the bounds (50) may reproduce $p_t$ even if $p_t$ is nonstationary. General conditions for nonsimultaneous equality in (50) can be derived from the proof of Proposition 1, i.e., from identifying the conditions for equality in Eqs. (36a) and (36b), using Theorem 1. We do not write down the general conditions because they involve the propagators and hence do not yield simple predictive criteria.

## V. 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 (50). 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

$$p_t \overset{\leqslant}{\geqslant} \sin^2_*\left( \arcsin\sqrt{\mathrm{tr}(\tilde{P}_t\rho_0)} \pm\hbar^{-1}\min\left\{ \int_0^t f(\tilde{P}_t,\tilde{H}_s)ds, \int_0^t f(\rho_0,\tilde{H}_s)ds \right\} \right), \tag{54}$$

$$\tilde{P}_t := W_t^* P W_t, \tag{55}$$

$$\tilde{H}_t := W_t^* H_t W_t - i\hbar W_t^* \dot{W}_t \tag{56}$$

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

$$p_t = \min_W T_+(t,\rho_0,P,W_\cdot) \tag{57a}$$

$$= \max_W T_-(t,\rho_0,P,W_\cdot) \tag{57b}$$

for all $t\geqslant 0$, where $T_\pm(t,\rho_0,P,W_\cdot)$ denotes the right-hand side of Eq. (54) as a function of $t$, $\rho_0$, $P$, and the family $W_\cdot$ [the dependence on $W_\cdot$ enters through (55) and (56)]. The minimum and maximum in Eq. (57) are attained when $W_s$ equals the exact propagator for all $0\leqslant s\leqslant t$. When $W_s=1$, for all $0\leqslant s\leqslant t$, Eq. (54) leads back to Eq. (50).

*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. (55), we wish to find a Hamiltonian $\tilde{H}_t$ such that the propagator $\tilde{U}_t$ generated by $\tilde{H}_t$ satisfies

$$\mathrm{tr}(P U_t\rho_0 U_t^*) = \mathrm{tr}(\tilde{P}_t\tilde{U}_t\rho_0\tilde{U}_t^*) \tag{58}$$

for all $\rho_0$ and $P$. The rationale is clear: The left-hand side of Eq. (58) equals $p_t$, and the right-hand side can be estimated by Eq. (50) with the replacement

$$\begin{aligned} &H_s \mapsto \tilde{H}_s, \\ &P \mapsto \tilde{P}_t \\ &p_t \mapsto \mathrm{tr}(\tilde{P}_t\tilde{U}_t\rho_0\tilde{U}_t^*), \\ &p_0 \mapsto \mathrm{tr}(\tilde{P}_t\rho_0). \end{aligned} \tag{59}$$

This yields Eq. (54) and exploits, as announced, the circumstance that the projection in Theorem 2 may be chosen $t$ dependent. It remains to find the Hamiltonian $\tilde{H}_t$ satisfying (58), i.e.,

$$U_t = W_t\tilde{U}_t, \tag{60}$$

$$i\hbar\dot{U}_t = H_t U_t, \tag{61}$$

$$i\hbar\dot{\tilde{U}}_t = \tilde{H}_t\tilde{U}_t. \tag{62}$$

Equation (60) follows from substituting (55) into (58). The other two equations are the evolution equations for the propagators $U_t$ and $\tilde{U}_t$. Substitution of Eq. (60) into (61) gives

$$\begin{aligned} H_t W_t\tilde{U}_t &= i\hbar\dot{W}_t\tilde{U}_t + i\hbar W_t\dot{\tilde{U}}_t, \\ &= i\hbar\dot{W}_t\tilde{U}_t + W_t\tilde{H}_t\tilde{U}_t, \end{aligned} \tag{63}$$

where Eq. (62) has been used in the second line. Multiplication of (63) by $W_t^*$ from the left and by $\tilde{U}_t^*$ from the right yields formula (56) for the transformed Hamiltonian $\tilde{H}_t$. We note that $\tilde{H}_t$ is formally self-adjoint, by the unitarity of $W_t$, for the latter implies that $W_t^*\dot{W}_t = -\dot{W}_t^* W_t$. If the trial propagator equals the exact propagator, $W_t=U_t$, then

$$\tilde{H}_t = U_t^* H_t U_t - i\hbar U_t^*(i\hbar)^{-1} H_t U_t = 0 \tag{64}$$

from Eqs. (56) and (61). Thus if $W_s=U_s$ for all $0\leqslant s\leqslant t$, the $\pm$ part in Eq. (54) vanishes, and (54) holds as an equality. This proves Eq. (57) and the statement about the attainment of the minimum and maximum. Finally, Eq. (50) is clearly a special case of (54). □

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

$$W_t \leftrightarrow \text{“free” propagator},$$

$\tilde{P}_t \leftrightarrow$ "free" Heisenberg evolution of $P$,

$\tilde{H}_t \leftrightarrow$ Hamiltonian in the "interaction picture."

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 Eq. (56). All that is needed for (54) is that $\tilde{P}_t$ and $\tilde{H}_t$ can be explicitly computed for a given $W_t$. The bounds (54) may then be interpreted as estimating $p_t$ in terms of the evolution of $P$ or $\rho_0$ under $W_t$, plus a correction term involving the Hamiltonian $\tilde{H}_s$ $(0 \leqslant s \leqslant t)$.

The fact that the family $W_\cdot$ is arbitrary converts inequality (54) into a variational principle. Indeed, since $W_\cdot$ occurs only on the right-hand side of (54), one may vary $W_\cdot$, so as to make the upper bound minimal or the lower bound maximal. When $W_\cdot$ is varied over all one-parameter families of unitary operators, the exact value of $p_t$ is obtained [Eqs. (57a) and (57b)]. Our variational principle provides explicit error estimates: For every $W_\cdot$, 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 $\rho_t$ may be written in the symmetric form

$$|\arcsin\sqrt{\mathrm{tr}(P\tilde{\rho}_t)} - \arcsin\sqrt{\mathrm{tr}(P\rho_t)}| \leqslant \hbar^{-1} \min\left\{ \int_0^t f(\tilde{P}_t, \tilde{H}_s)\,ds, \int_0^t f(\rho_0, \tilde{H}_s)\,ds \right\}, \tag{65}$$

which is equivalent to Eq. (54) and puts the error bound into full evidence. Thus, if $W_\cdot$ is a good approximation of $U_\cdot$, then $\tilde{H}_s$ will be small and the bounds (54) will bracket $p_t$ tightly, even when $t$ is large. Conversely, if $W_\cdot$ is a poor approximation of $U_\cdot$, then the upper and lower bounds will be close to each other only for small $t$ and will rapidly approach 1 and 0 as $t$ grows. The dependence of Eq. (54) on the cumulative energy uncertainties reflects the fact that the bounds (54) measure the performance of the whole family $W_\cdot$, not just of a single operator $W_t$.

It may happen that, for given $W_\cdot, P, \rho_0$, the bounds (54) coincide and thus produce the exact value $p_t$ even if $W_s \neq U_s$ for all $0 < s \leqslant t$ ("perfect performance of a wrong family"). An elementary example is the trivial guess, $W_s = 1$ for $0 \leqslant s \leqslant t$, which gives the exact value $p_t$ whenever $P$ or $\rho_0$ is a constant of motion (Theorem 2). It shows that the family $W_\cdot$, which minimizes and maximizes the functionals $T_\pm(t, \rho_0, P, \cdots)$, need not be unique. The origin of this degeneracy is that two different families, $W_\cdot$ and $\overline{W}_\cdot$, may act identically on $P$ or $\rho_0$,

$$W_t^* P W_t = \overline{W}_t^* P \overline{W}_t, \tag{66a}$$

$$W_t \rho_0 W_t^* = \overline{W}_t \rho_0 \overline{W}_t^*, \tag{66b}$$

in which case they may perform identically in Theorem 3. Thus one may get a good estimate of $p_t$ from a single guess $W_\cdot$; and the estimate of $p_t$ may be good even if $W_\cdot$ is far from the exact time evolution $U_\cdot$.

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 Eq. (65). 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. (65), for the difference between the trial state and the exact state.

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

**Corollary 1**. Consider a system with a family of time-dependent Hamiltonians $H_t$, a solution $\psi_t$ 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 $\varphi$ and all $t \geqslant 0$, one has the bounds

$$|\langle\varphi|\psi_t\rangle| \begin{matrix} \leqslant \\ \geqslant \end{matrix} \sin_*\left( \arcsin|\langle\varphi|\tilde{\psi}_t\rangle| \pm \hbar^{-1} \int_0^t \|(1 - |\tilde{\psi}_s\rangle\langle\tilde{\psi}_s|)\,\delta(\tilde{\psi}_s)\|\,ds \right), \tag{67a}$$

$$1 \geqslant |\langle\tilde{\psi}_t|\psi_t\rangle| \geqslant \cos_*\left( \hbar^{-1} \int_0^t \|(1 - |\tilde{\psi}_s\rangle\langle\tilde{\psi}_s|)\,\delta(\tilde{\psi}_s)\|\,ds \right), \tag{67b}$$

where

$$\delta(\tilde{\psi}_s) := H_s\tilde{\psi}_s - i\hbar\dot{\tilde{\psi}}_s,$$

$$\cos_*(x) := \sqrt{1 - \sin_*^2(x)}.$$

Equality holds in (67) if and only if there exist real numbers $a_s$ such that $\tilde{\psi}_s = e^{ia_s}\psi_s$, for all $0 \leqslant s \leqslant t$.

*Proof.* We write the trial states as

$$\tilde{\psi}_t = W_t\psi_0, \tag{68}$$

where $W_\cdot$ is a family satisfying the hypotheses of Theorem 3. For a given trial-state family $\tilde{\psi}_\cdot$, the propagator family $W_\cdot$ 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

$$f^2(\tilde{P}_t, \tilde{H}_s) = \|\tilde{H}_s W_t^*\varphi\|^2 - \langle W_t^*\varphi|\tilde{H}_s W_t^*\varphi\rangle^2, \tag{69}$$

$$\begin{aligned} f^2(\rho_0, \tilde{H}_s) &= \|\tilde{H}_s\psi_0\|^2 - \langle\psi_0|\tilde{H}_s\psi_0\rangle^2 \\ &= \|(1 - |\psi_0\rangle\langle\psi_0|)\tilde{H}_s\psi_0\|^2 \\ &= \|W_s(1 - |\psi_0\rangle\langle\psi_0|)W_s^*(H_sW_s - i\hbar\dot{W}_s)\psi_0\|^2 \\ &= \|(1 - |\tilde{\psi}_s\rangle\langle\tilde{\psi}_s|)\,\delta(\tilde{\psi}_s)\|^2 \\ &= \|\delta(\tilde{\psi}_s)\|^2 - |\langle\tilde{\psi}_s|\,\delta(\tilde{\psi}_s)\rangle|^2, \end{aligned} \tag{70}$$

where Eqs. (52), (55), (56), (68), unitarity of $W_s$, and the definition of $\delta(\tilde{\psi}_s)$ have been used. Since the energy uncertainty (69) cannot be expressed in terms of the trial states, we

keep only the term $f(\rho_0,\tilde{H}_s)$ in Eq. (54), at the expense of weakening the bounds. This gives the result (67a) from (70). The result (67b) follows from (67a) by choosing the reference state equal to the trial state, $\varphi=\tilde{\psi}_t$. Equality holds in Eq. (67) if and only if, for all $0\leqslant s\leqslant t$, 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. □

We now discuss Corollary 1. (i) Intuitively, a trial state $\tilde{\psi}_t$ is a good approximation of the solution $\psi_t$ 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 $\psi_t$ in terms of $\tilde{\psi}_s$, which are manifestly tight if $\delta(\tilde{\psi}_s)$ is small ($0\leqslant s\leqslant t$). 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 (67) are tight whenever $\delta(\tilde{\psi}_s)$ lies almost in the subspace spanned by $\tilde{\psi}_s$.

(ii) The result (67) 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 end point $t$, but the one that minimizes (in the sense of the above norm) the cumulative remainder over $0\leqslant s\leqslant t$. This agrees with the earlier remark that our variational bounds measure the performance of a one-parameter family, here $\tilde{\psi}_\cdot$, rather than of a single element, $\tilde{\psi}_t$.

(iii) Once the best family has been identified and the integral in (67) has been evaluated, the bounds (67a) give estimates of the overlap of the exact state $\psi_t$ and any vector $\varphi$. This provides a complete catalog of error estimates for the location of $\psi_t$ in $\mathscr{H}$. The error estimate for the location of $\psi_t$ relative to $\tilde{\psi}_t$ is given by Eq. (67b). Upon introduction of a suitable phase factor $e^{ia_t}$, the estimate (67b) can also be put in the form

$$\|\psi_t-e^{ia_t}\tilde{\psi}_t\|=(2-2|\langle\psi_t|\tilde{\psi}_t\rangle|)^{1/2}\leqslant 2\sin_*\left(\frac{1}{2}\hbar^{-1}\int_0^t\|(1-|\tilde{\psi}_s\rangle\langle\tilde{\psi}_s|)\,\delta(\tilde{\psi}_s)\|\,ds\right). \tag{71}$$

The bound (71) may be used to reestimate the overlap of $\psi_t$ and $\varphi$ from

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

and the Schwarz inequality. But the resulting estimate for $|\langle\varphi|\psi_t\rangle|$ is weaker than (67a), as shown by Eq. (53a).

(iv) If a trial-state family comes from a known trial-propagator family, Eq. (68), or if, conversely, a given trial-state family is extended to a trial-propagator family, the bounds (67a) can be improved by including the omitted term (69). This will be further discussed in Sec. VI. No such improvement is possible in (67b) because, for $\varphi=\tilde{\psi}_t$, Eqs. (69) and (70) yield $f(\tilde{P}_t,\tilde{H}_s)=f(\rho_0,\tilde{H}_s)$, i.e., identical results. Thus the bound (67b) 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 Eq. (67) is a variational principle for one-dimensional subspaces of $\mathscr{H}$, rather than vectors in $\mathscr{H}$. 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 (67a) is unique. The nonuniqueness of the minimizing and maximizing family $W_\cdot$ in Theorem 3 disappears in Corollary 1 because when we consider a specific family of density operators $W_t\rho_0W_t^*$, as we do in Corollary 1, the degeneracy (66) is automatically lifted.

## VI. 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 (1973) and Bhattacharyya (1983) showed that the solution $\psi_t$ of (2b) satisfies

$$|\langle\psi_0|\psi_t\rangle|\geqslant\cos_*((\langle\psi_0|H^2\psi_0\rangle-\langle\psi_0|H\psi_0\rangle^2)^{1/2}t/\hbar). \tag{72}$$

This is the lower bound (50) and (51) for the special case $P=\rho_0=|\psi_0\rangle\langle\psi_0|$, recalling (52) and noting that (50) and (51) coincide if the Hamiltonian is time independent. It is also the bound (67b) for the special case in which the trial family is $\tilde{\psi}_s=\psi_0$, $0\leqslant s\leqslant t$, with remainder $\delta(\tilde{\psi}_s)=H\psi_0$. The result (72) was used by Fleming (1973) and Bhattacharyya (1983) to deduce the bound (5) for the half-life time $\tau_2$ and the death time $\tau_3$ of the initial state $\psi_0$.

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 (50) and (51), with (52), were obtained by Pfeifer (1993), 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 Pfeifer, 1994). It was claimed in Pfeifer, 1993, that the bounds (51) hold without restrictions, under the condition that $P$ and $\rho_0$ have rank one. But we have found a gap in the arguments for that claim. So at present Eq. (51) is established only if the Hamiltonians at different times commute with each other. All other assertions in Pfeifer, 1993, 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 $\psi_t$ in terms of the trial states $\tilde{\psi}_s$. All previous time-dependent variational principles for state vectors approximate $\psi_t$ by an extremalized trial state $\tilde{\psi}_t$, without error estimates (see Gerjuoy, Rau, and Spruch, 1983; Pfeifer and Levine, 1983; Broeckhove, Lathouwers, and van Leuven, 1989, for some complementary reviews). One such popular principle, attributed to McLachlan (Broeckhove, Lathouwers, and van Leuven, 1989; McLachlan, 1964), minimizes the norm of the vector $\delta(\tilde{\psi}_t)$ defined in Corollary 1. It provides no error bars because the Schrödinger equation alone gives no information

about the closeness of $\tilde{\psi}_t$ to $\psi_t$ when $\|\delta(\tilde{\psi}_t)\|$ is small. 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 with error bounds. Spruch (1969) derived upper and lower bounds for the overlap of the solution $\psi_t$ of (2b) and any reference state $\varphi$ that amount to

$$|\langle\varphi|\psi_t\rangle| \overset{\leqslant}{\geqslant} |\langle\varphi|W_t\psi_0\rangle| \pm \hbar^{-1}\int_0^t \|(H_sW_s - i\hbar\dot{W}_s)W_t^*\varphi\|ds, \tag{73}$$

for a trial-propagator family $W_\cdot$ as in Theorem 3. Spruch's bounds [Eq. (73)] 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 Eq. (54), we obtain

$$\begin{aligned}|\langle\varphi|\psi_t\rangle| &\overset{\leqslant}{\geqslant} \sin_*\left(\arcsin|\langle\varphi|W_t\psi_0\rangle| \pm \hbar^{-1}\int_0^t f(\tilde{P}_t,\tilde{H}_s)ds\right)\\ &\overset{\leqslant}{\geqslant} |\langle\varphi|W_t\psi_0\rangle| \pm \hbar^{-1}\int_0^t f(\tilde{P}_t,\tilde{H}_s)ds\\ &\overset{\leqslant}{\geqslant} |\langle\varphi|W_t\psi_0\rangle| \pm \hbar^{-1}\int_0^t \|\tilde{H}_sW_t^*\varphi\|ds.\end{aligned} \tag{74}$$

In the second line, we have used the inequality (53b); and in the third line, we have inserted Eq. (69), dropping its second term. By Eq. (56) and the unitarity of $W_s$, the third line is the same as Eq. (73).

This derivation of Eq. (73) from (54) 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 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 (1969) and Shakeshaft and Spruch (1974) derived additional bounds which, in the notation of (74), read

$$\begin{aligned}|\langle\varphi|\psi_t\rangle| &\overset{\leqslant}{\geqslant} \left|\left\langle\varphi|W_t\left(1-i\hbar^{-1}\int_0^t\tilde{H}_sds\right)\psi_0\right\rangle\right|\\ &\quad \pm\hbar^{-2}\int_0^t\|\tilde{H}_s\psi_0\|\int_s^t\|\tilde{H}_{s'}W_t^*\varphi\|ds'ds.\end{aligned} \tag{75}$$

In these bounds, the initial state is propagated by a nonunitary operator, $W_t(1-i\hbar^{-1}\int_0^t\tilde{H}_sds)$. 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 (74) and (75) are perturbation theoretic in nature (see also Spruch, 1969; Shakeshaft and Spruch, 1974); and so is Theorem 3. Indeed, returning to our analysis, we find that in Theorem 3 we have used nothing more than a variant of second-order, time-dependent perturbation theory (Dyson series for $U_tW_t^*$ 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 $\rho_0$. A similar comparison dynamics is required in Spruch, 1969, and Shakeshaft and Spruch, 1974, except that there the subspace is one dimensional.

Our methods are reminiscent of Nekhoroshev's perturbation theory in classical mechanics (Nekhoroshev, 1977). 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 Nekoroshev-type methods (Benettin, Galgani, and Giorgilli, 1987, 1989; Benettin, Fröhlich, and Giorgilli, 1988), although our systems will be very different from those studied by Benettin *et al.* (Benettin, Galgani, and Giorgilli, 1987, 1989; Benettin, Fröhlich, and Giorgilli, 1988). Actually, all results proven in Secs. III–V 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.

## VII. 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 by Pfeifer (1993). 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 (54) for carefully chosen comparison dynamics.

### A. 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 $v_\theta$, with

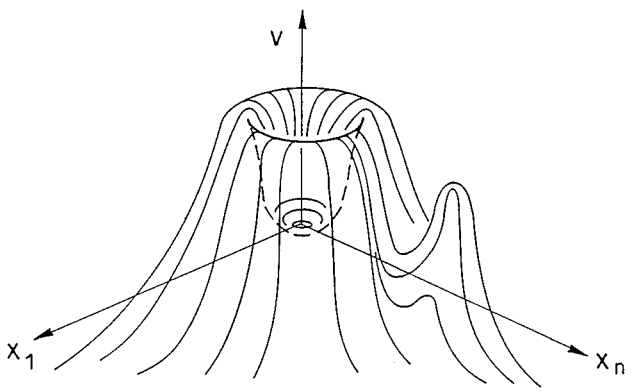


FIG. 1.

$$v_\theta(\boldsymbol{x}) := \theta^2 v(\boldsymbol{x}/\theta), \quad 1 \leqslant \theta < \infty, \tag{76}$$

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

(i) The origin $\boldsymbol{x}=0$ is a local minimum of $v$, with $v(0)=0$.

(ii) The Hessian of $v$ at $\boldsymbol{x}=0$ is positive-definite, with eigenvalues $\Omega_i^2 > 0$, $i=1, \ldots, n$.

(iii) Let $g(\boldsymbol{x})$ be a smooth function, with $g(\boldsymbol{x})=1$, for $|\boldsymbol{x}| \leqslant \frac{1}{2}$, and $g(\boldsymbol{x})=0$, for $|\boldsymbol{x}| \geqslant 1$.

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

$$g_{\varepsilon,\theta}(\boldsymbol{x}) := g\left(\frac{\boldsymbol{x}}{(\varepsilon\theta)^{1/3}}\right), \quad \varepsilon > 0. \tag{77}$$

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

$$\max_{\boldsymbol{x}} g_{\varepsilon,\theta}(\boldsymbol{x}) \left| v_\theta(\boldsymbol{x}) - \frac{1}{2}\sum_{i=1}^{n} \Omega_i^2 x_i^2 \right| \leqslant c_1 \varepsilon, \tag{78}$$

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

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

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

The Hilbert space of the system is given by

$$\mathscr{H} = L^2(\mathbb{R}^n, d^n x), \tag{79}$$

and the Hamiltonian is

$$H \equiv H_\theta := -\frac{\hbar^2}{2m}\Delta + v_\theta(\boldsymbol{x}), \tag{80}$$

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

$$H_1 \equiv H_{1,\theta} := H_0 + w_{\varepsilon,\theta}(\boldsymbol{x}), \tag{81}$$

where

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

$$w_{\varepsilon,\theta}(\boldsymbol{x}) = g_{\varepsilon,\theta}(\boldsymbol{x})\left[ v_\theta(\boldsymbol{x}) - \frac{1}{2}\left(\sum_{i=1}^{n} \Omega_i^2 x_i^2\right)\right]. \tag{82}$$

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 Eq. (82). With the units and conventions just fixed, the spectrum of $H_0$ consists of the eigenvalues

$$E_{\boldsymbol{l}} = \sum_{i=1}^{n} \Omega_i \left( l_i + \frac{1}{2}\right), \tag{83}$$

where $\boldsymbol{l} = (l_1, \ldots, l_n)$, and $l_i = 0, 1, 2, \ldots$ for $i = 1, \ldots, n$, corresponding to the eigenfunctions

$$\psi_{\boldsymbol{l}}(\boldsymbol{x}) = \prod_{i=1}^{n} \Omega_i^{1/4} h_{l_i}(\sqrt{\Omega_i}\, x_i), \tag{84}$$

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

$$|h_l(x)| \leqslant c_{l,\delta} \exp\left[ -\left(\frac{1}{2} - \delta\right) x^2 \right], \tag{85}$$

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

$$E_{\boldsymbol{l}^{(j)}} < E \quad \text{for all } j = 1, \ldots, k_E, \tag{86}$$

with $k_E \leqslant a_n (E/\Omega_0)^n$, where $\Omega_0 := \min_i \Omega_i > 0$, and $a_n$ is a geometrical constant. Defining $|\boldsymbol{l}| := \max_i l_i$, we also have $|\boldsymbol{l}^{(j)}| < \Omega_0^{-1} E$ for all $j = 1, \ldots, k_E$.

We may view the Hamiltonian $H_1$ as a perturbation of $H_0$ by the potential $w_{\varepsilon,\theta}(\boldsymbol{x})$. By Eqs. (78) and (82), the operator norm, $\|w_{\varepsilon,\theta}\|$, of $w_{\varepsilon,\theta}$ is bounded by $c_1\varepsilon$, and hence we can apply analytic perturbation theory (Kato, 1980). We choose a contour $\gamma_E$ in the complex plane surrounding (spec $H_0$) $\cap [0, E)$ such that

$$\text{dist}(\gamma_E, \text{spec } H_0) =: d_E = \frac{1}{2}(E_{\boldsymbol{l}^{(k_E+1)}} - E_{\boldsymbol{l}^{(k_E)}}) > 0. \tag{87}$$

We choose $\varepsilon$ so small that

$$c_1 \varepsilon \leqslant \frac{d_E^2}{3(E + \Omega_0)}. \tag{88}$$

Then the operator

$$P_{\theta,E} = \frac{1}{2\pi i} \oint_{\gamma_E} dz\, (z - H_1)^{-1} \tag{89}$$

is a spectral projection of $H_1$, with

$$\text{tr}(P_{\theta,E}) = k_E \quad \text{and} \quad \|P_{\theta,E} - P_E^0\| < 1, \tag{90}$$

where $P_E^0$ is the spectral projection of $H_0$ onto the subspace, $\mathscr{H}_E$, spanned by the eigenfunctions $\{\psi_{\boldsymbol{l}^{(1)}}, \ldots, \psi_{\boldsymbol{l}^{(k_E)}}\}$.

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

$$\|e^{\alpha|\boldsymbol{x}|^2}\psi\| \leqslant C_E \|\psi\|, \tag{91}$$

provided $\alpha > 0$ is sufficiently small (depending on $\varepsilon$ and $C_E$). This follows from a Combes-Thomas argument (Combes and Thomas, 1973; see also Hunziker, 1977): First, we note that, by Eq. (90), there is a vector $\varphi \in \mathscr{H}_E$ such that $\psi = P_{\theta,E}\varphi$, with $\|\varphi\| \leqslant \text{const}\, \|\psi\|$. Using Eq. (89), we have

$$e^{\alpha|\boldsymbol{x}|^2}\psi = \frac{1}{2\pi i} \oint_{\gamma_E} dz \{e^{\alpha|\boldsymbol{x}|^2}(z - H_1)^{-1} e^{-\alpha|\boldsymbol{x}|^2}\} e^{\alpha|\boldsymbol{x}|^2}\varphi. \tag{92}$$

By Eqs. (84)–(86),

$$\|e^{\alpha|\boldsymbol{x}|^2}\varphi\| \leqslant \text{const}\, \|\varphi\|,$$

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

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

where

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

Choosing $\alpha$ small enough, we can use elementary analytic perturbation theory (Kato, 1980) to prove a uniform bound on

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

for all $z\in\gamma_E$. From this and Eq. (92) the bound (91) follows by standard arguments.

Finally, we note that

$$H-H_1=\delta v_{\varepsilon,\theta}, \tag{93}$$

where

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

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),

$$|\delta v_{\varepsilon,\theta}(x)|\leq\begin{cases}0, & |x|\leq\frac{1}{2}(\varepsilon\theta)^{1/3},\\ a\theta^2+b|x|^2+P(x)/\theta, & |x|>\frac{1}{2}(\varepsilon\theta)^{1/3},\end{cases} \tag{94}$$

for some finite constants $a$ and $b$ and some polynomial $P(x)$.

With these preliminaries out of the way, we are ready to apply the bounds (54) on the probability $p_t$ (see Theorem 3) to the present system. The system is in an initial state described by a density matrix $\rho_0$. Given some number $\sigma$, $0<\sigma<1$, there then exists an energy $E_\sigma<\infty$ such that

$$\mathrm{tr}(\rho_0P_{\theta,E})\geq(1-\sigma)^2, \tag{95}$$

for all $E\geq E_\sigma$ and all $\theta\geq1$. This follows easily from the definition (89) of the projection $P_{\theta,E}$, Eqs. (81) and (84), and assumption (iii) [Eq. (78)].

We now set

$$U_t=e^{-itH},\quad W_t=e^{-itH_1},$$

$$\tilde{P}_t=W_t^*P_{\theta,E}W_t=P_{\theta,E}, \tag{96}$$

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. (81)]. We then have [see Eq. (56)]

$$\begin{aligned}\tilde{H}_t&=W_t^*HW_t-iW_t^*\dot{W}_t\\&=W_t^*\delta v_{\epsilon,\theta}W_t,\end{aligned} \tag{97}$$

by Eqs. (96) and (93).

Using Eqs. (30b), (96), and (97), we find that

$$\begin{aligned}f(\tilde{P}_t,\tilde{H}_s)&=f(W_{t-s}^*P_{\theta,E}W_{t-s},\delta v_{\varepsilon,\theta})\\&=f(P_{\theta,E},\delta v_{\varepsilon,\theta}),\end{aligned} \tag{98}$$

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

Equation (II.3b) (Table II) says that

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

We may represent $P_{\theta,E}$ as an integral operator on $\mathscr{H}$, with integral kernel denoted by $\Pi_{\theta,E}(x,y)$. By Eqs. (90) and (91), we have

$$\int|\Pi_{\theta,E}(x,y)|^2e^{2\alpha(|x|^2+|y|^2)}d^nxd^ny\leq(k_EC_E)^2, \tag{99}$$

with $C_E$ and $\alpha$ as specified in Eq. (91), and $k_E$ as in (86). Furthermore,

$$\begin{aligned}\mathrm{tr}(-[P_{\theta,E},\delta v_{\varepsilon,\theta}]^2)=\int|\Pi_{\theta,E}(x,y)|^2[\,&\delta v_{\varepsilon,\theta}(x)\\&-\delta v_{\varepsilon,\theta}(y)]^2d^nxd^ny.\end{aligned} \tag{100}$$

Recalling inequality (94) and using (99), we conclude that

$$0\leq\mathrm{tr}(-[P_{\theta,E},\delta v_{\varepsilon,\theta}]^2)\leq2\delta_E^2e^{-2\mu_E\theta^{2/3}}, \tag{101}$$

for some finite constants $\delta_E$ and $\mu_E$ that depend on $E$. [Here $\mu_E\propto\alpha\varepsilon^{2/3}$, and, by Eqs. (91) and (88), $\alpha$ and $\varepsilon$ depend on $E$.]

With

$$\rho_t:=U_t\rho_0U_t^*\ \text{ and }\ p_t:=\mathrm{tr}(\rho_tP_{\theta,E}), \tag{102}$$

inequality (54) of Theorem 3, combined with inequality (95), Eq. (98), and inequality (101), yields the bounds

$$p_t\ \begin{matrix}\leq\\ \geq\end{matrix}\ \sin_*^2\left(\arcsin(1-\sigma)\pm\int_0^tf(\tilde{P}_t,\tilde{H}_s)ds\right),$$

where

$$\begin{aligned}0\leq f(\tilde{P}_t,\tilde{H}_s)&=\sqrt{\tfrac{1}{2}\,\mathrm{tr}(-[P_{\theta,E},\delta v_{\varepsilon,\theta}]^2)}\\&\leq\delta_Ee^{-\mu_E\theta^{2/3}},\end{aligned} \tag{103}$$

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

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

and we find that

$$p_t\ \begin{matrix}\leq\\ \geq\end{matrix}\ \sin_*^2\left(\frac{\pi}{2}-\sqrt{2^{\mp1}\sigma}\ \pm\ t\,\delta_Ee^{-\mu_E\theta^{2/3}}\right), \tag{104}$$

for $\sigma$ small enough and $E\geq E_\sigma$. These bounds imply that the state $\rho_t$ of the system remains in the range of the spectral projection $P_{\theta,E}$ of the operator $H_{1,\theta}$ [defined in Eq. (81)], for $E$ large enough, with *positive probability* $p_t$ [estimated by Eq. (104)], *for all times* $t$, with

$$|t|<\mathrm{const}\,e^{\mu_E\theta^{2/3}}. \tag{105}$$

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 $\mathscr{H}$ 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

$$\|(1-Q_R)P_{\theta,E}\|\leq\beta, \tag{106}$$

for all $R>R_{E,\beta}$. This is an easy consequence of inequality (99). From (106) one obtains

$$p_t = \mathrm{tr}(P_{\theta,E}\rho_t) = \mathrm{tr}(Q_R P_{\theta,E}\rho_t) + \mathrm{tr}((1-Q_R)P_{\theta,E}\rho_t)$$
$$\leq \mathrm{tr}(Q_R P_{\theta,E}\rho_t) + \beta$$
$$= q_t + \mathrm{tr}(Q_R(P_{\theta,E}-1)\rho_t) + \beta$$
$$\leq q_t + \sqrt{q_t}\sqrt{1-p_t} + \beta, \tag{107}$$

where, in the first inequality we have used (106), we have defined $q_t$ by

$$q_t := \mathrm{tr}(\rho_t Q_R), \tag{108}$$

and in the last inequality we have used the cyclicity of the trace and the Schwarz inequality for the trace and have noted that $\mathrm{tr}((P_{\theta,E}-1)^2\rho_t) = \mathrm{tr}((1-P_{\theta,E})\rho_t) = 1-p_t$. From Eqs. (104), (107), and (106) we conclude that, *for R large enough* ($R > R_{E,\beta}, E \geq E_\sigma, \beta$ and $\sigma$ small enough),

$$q_t \geq \frac{1}{2}, \text{ for all } t \text{ with } |t| < \text{const } e^{\tilde{\mu}_R \theta^{2/3}}, \tag{109}$$

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 $v_\theta$), does not escape from it, for all times $t$ with

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

We discuss this result as follows. (1) Let us suppose that the function $v$ is $C^4$ and has *vanishing* third derivatives at its local minimum $\boldsymbol{x}=0$ [this has *not* been assumed in the analysis presented above; see Eq. (78)]. In this case, we redefine the function $g_{\varepsilon,\theta}(\boldsymbol{x})$ [see Eq. (77)] by setting

$$g_{\varepsilon,\theta}(\boldsymbol{x}) := g\left(\frac{\boldsymbol{x}}{\sqrt{\varepsilon\,\theta}}\right), \tag{110}$$

with $\varepsilon$ small enough. Under the present hypotheses, inequality (78) holds for the function $g_{\varepsilon,\theta}$ defined in Eq. (110). Going through our analysis step by step, we then find that inequality (101) can be improved to

$$0 \leq \mathrm{tr}(-[P_{\theta,E}, \delta v_\theta]^2) \leq 2\,\delta_E^2 e^{-2\mu_E \theta}, \tag{101'}$$

and (109) turns out to hold *for all times t with*

$$|t| \leq \exp[\text{const } \theta], \tag{111}$$

i.e., *for exponentially large times*.

One may wonder whether Eq. (111) can be improved, under suitable assumptions on $v$, to superexponentially large times. Actually, it is easy to see that if $v(\boldsymbol{x}) \to \text{const}$, as $|\boldsymbol{x}| \to \infty$ (i.e., the "volcano" does not permanently confine the particle), Eq. (111) cannot be improved without changing the comparison dynamics. This is seen by carefully retracing the steps of our analysis. In order to improve on Eq. (111), one would have to use a comparison dynamics involving a potential that grows faster than $|\boldsymbol{x}|^2$ as $|\boldsymbol{x}| \to \infty$. 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 $v_\theta$: One sets

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

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

$$g_\varepsilon(\boldsymbol{x}) := g(\boldsymbol{x}/\varepsilon)$$

and set

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

We assume that

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

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

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

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

$$H_1 := H_0 + w_{\varepsilon,\theta}$$

and

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

where

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

Then the spectrum of $H_0$ consists of the eigenvalues

$$E_{\boldsymbol{l}} = \sum_{i=1}^n \theta\Omega_i(l_i + \tfrac{1}{2}), \quad l_i = 0,1,2,\ldots, \quad i = 1,\ldots,n,$$

corresponding to the eigenfunctions

$$\psi_{\boldsymbol{l}}(\boldsymbol{x}) = \prod_{i=1}^n (\theta\Omega_i)^{1/4} h_{l_i}(\sqrt{\theta\Omega_i}\,x_i),$$

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

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

for all $\psi$ 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 $E = \mathscr{E}\theta$, $\mathscr{E} < \infty$, for $\varepsilon$ sufficiently small. The Combes-Thomas argument [see (91) and (92)] can be used, just as before, to show that the corresponding eigenfunctions of $H_1$ decay like $\exp[-\alpha_{\mathscr{E}}\theta|\boldsymbol{x}|^2]$ for some $\alpha_{\mathscr{E}} > 0$. Let $P_{\mathscr{E}}$ denote the spectral projection of $H_1$ onto the subspace spanned by eigenfunctions corresponding to eigenvalues $\leq \mathscr{E}\theta$. Preparing the system in a state $\rho_0$ with the property that

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

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

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

for some $\mu_{\mathscr{E}} > 0$. As in Eqs. (106)–(109), 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 $\rho_0$ described above, is exponentially large in $\theta$.

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

For discussion of and references to other related results see Cycon, Froese, Kirsch, and Simon (1987).

### B. 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. At time $t=0$, the nucleus and the electron are supposed to form a bound state; the initial state $\rho_0$ 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 $\chi_0$ for the center-of-mass motion is assumed to be peaked at a point $\vec{X}_0=(r,0,0)$, and its Fourier transform $\hat{\chi}_0$ to be peaked at a momentum given by $\vec{P}_0=M\vec{V}_0$, where $\vec{V}_0=(0,-r\omega_c,0)$, and $\omega_c$ is the cyclotron angular velocity of a particle of electric charge $q=Ze$ and mass $M$, i.e.,

$$\omega_c=\frac{qB}{Mc}. \tag{112}$$

By Heisenberg's uncertainty relations,

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

If $Z$ is large, $M$ 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

$$\Omega:=\begin{pmatrix} 0 & \omega_c & 0 \\ -\omega_c & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \tag{113}$$

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*

$$\vec{y}=e^{-\Omega t}\vec{x} \tag{114}$$

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

$$\vec{V}(\vec{y})=\frac{d}{dt}(e^{-\Omega t}\vec{x})=-\Omega\vec{y}. \tag{115}$$

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

$$-\frac{(Z+1)e^2}{|\vec{x}-\vec{X}(t)|}=-\frac{(Z+1)e^2}{|\vec{y}-\vec{X}_0|}=:v_c(\vec{y}). \tag{116}$$

Thus, in moving coordinates $\vec{y}$ [given by Eq. (114)], $v_c(\vec{y})$ 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 by Fröhlich and Studer (1993). 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 $\phi_t$ on $\mathbb{R}^3$ [i.e., $(\partial/\partial t)\phi_t(\vec{y})=\vec{V}(\phi_t(\vec{y}),t)$ with $\vec{\nabla}\cdot\vec{V}=0$]. 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 $\psi_t$ is a two-component Pauli spinor, with

$$\psi_t \in \mathscr{H} := L^2(\mathbb{R}^3,d^3y)\otimes\mathbb{C}^2 \tag{117}$$

and

$$H_y=\left\{\frac{1}{2m_*}\left(\frac{\hbar}{i}\vec{\nabla}+\frac{e}{c}\vec{A}-m_*\vec{V}\right)^2+v_c-\frac{e}{c}\vec{V}\cdot\vec{A}-\frac{m_*}{2}\vec{V}^2\right\}\otimes 1_2+1\otimes\left\{-\frac{g\mu}{\hbar}\vec{B}\cdot\vec{S}+2\vec{\omega}\cdot\vec{S}\right\}, \tag{118}$$

where $m_*=mM/(m+M)\approx m$ is the reduced mass of the electron, $g\approx 2$ is its gyromagnetic factor, $\mu=e\hbar/(2mc)$ is the Bohr magneton, $\vec{S}=(\hbar/2)(\sigma_x,\sigma_y,\sigma_z)$ is the spin operator of the electron, and $\vec{\omega}=\frac{1}{2}\,\mathrm{curl}\,\vec{V}$ [with $\vec{\omega}=(0,0,\omega_c)$, $\omega_c$ as in Eq. (112), in our example] is the angular velocity of the moving coordinate frame. The first term on the right-hand side of Eq. (118) is the kinetic-energy operator in moving coordinates, with $m_*\vec{V}$ corresponding to the vector potential of the Coriolis force; the term $-(e/c)\vec{V}\cdot\vec{A}$ is a relativistic correction, due to the circumstance that, in moving coordinates, there is an electric field proportional to $(|\vec{V}|/c)|\vec{B}|$; the term $-(m_*/2)\vec{V}^2$ is the potential of the centrifugal force; the term $-(g\mu/\hbar)\vec{B}\cdot\vec{S}$ 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 right-hand side of Eq. (118) are expressed in the basis of the moving frame. For simplicity we are neglecting spin-orbit interactions in Eq. (118) which, for large $Z$ are actually somewhat significant. For details concerning the derivation of Eq. (118), see Fröhlich and Studer (1993).

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

$$\vec{A}(\vec{y})=\frac{B}{2}(-y_2,y_1,0), \tag{119}$$

and, by Eqs. (113) and (115),

$$\vec{V}(\vec{y})=\omega_c(-y_2,y_1,0). \tag{120}$$

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

$m_*/M \ll 1$, $B_*$ is approximately equal to $B$. Furthermore, approximating $g$ by 2 and $m_*$ by $m$, we find that

$$-\frac{g\mu}{\hbar}\vec{B}\cdot\vec{S}+2\vec{\omega}\cdot\vec{S}\approx-\frac{g\mu}{\hbar}\vec{B}_*\cdot\vec{S}. \tag{121}$$

Actually, the fact that (121) is not a strict equation is significant and is the basis of Telegdi's precision experiment determining the $g$ factor of the electron. For our considerations, however, the deviation of the left-hand side from the right-hand side of Eq. (121) is insignificant.

Finally,

$$\left[-\frac{e}{c}\vec{A}\cdot\vec{V}-\frac{m_*}{2}\vec{V}^2\right](\vec{y})=-\frac{(qB)^2}{2Mc^2}\left(\frac{e}{q}+\frac{m_*}{M}\right)(y_1^2+y_2^2)$$
$$\approx-\frac{eqB_*^2}{2Mc^2}(y_1^2+y_2^2), \tag{122}$$

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

All these calculations show that

$$H_y\approx\left\{\frac{1}{2m_*}\left(\frac{\hbar}{i}\vec{\nabla}+\frac{e}{c}\vec{A}_*\right)^2-\frac{eq}{|\vec{y}-\vec{X}_0|}-\frac{eqB_*^2}{2Mc^2}(y_1^2+y_2^2)\right\}$$
$$\otimes 1_2-1\otimes\frac{g\mu}{\hbar}\vec{B}_*\cdot\vec{S}. \tag{123}$$

The terms left out on the right-hand side give corrections of order $Em/M$ to a typical energy $E\in$ spec $H_y$. Consideration of the right side of (123) suggests that we use relative coordinates

$$\vec{\xi}:=\vec{y}-\vec{X}_0=(y_1-r,y_2,y_3). \tag{124}$$

Then

$$-\frac{eqB_*^2}{2Mc^2}(y_1^2+y_2^2)+\frac{eqB_*^2}{2Mc^2}r^2=-\frac{eqB_*^2}{Mc^2}r\xi_1$$
$$-\frac{eqB_*^2}{2Mc^2}(\xi_1^2+\xi_2^2). \tag{125}$$

The Bohr radius $a$ is many orders of magnitude smaller than $r$, which, in a cyclotron, is macroscopically large. Thus the second term on the right-hand side of Eq. (125) is, for all practical purposes, negligible. The size of the first term is

$$\left|\frac{eqB_*^2}{Mc^2}r\xi_1\right|\sim\frac{eqB_*^2}{Mc^2}ra$$
$$\ll\frac{q^2B^2}{2Mc^2}r^2=\frac{M}{2}(\omega_c r)^2. \tag{126}$$

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

$$\vec{E}_*=\left(\frac{qB_*^2}{Mc^2}r,0,0\right), \tag{127}$$

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 tunneling in atomic physics: Let $\mathscr{H}$ be as in Eq. (117), 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. (77). Let $v$ be a piecewise continuous function on $\mathbb{R}^3$ with the following properties: We define

$$w_\theta(\vec{\xi}):=g\left(\frac{\vec{\xi}}{\theta}\right)v(\vec{\xi}), \tag{128}$$

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

$$\|w_\theta\psi\|\leq\Lambda_\theta\|(H_0+k1)\psi\|, \tag{129}$$

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

$$\delta v_\theta(\vec{\xi}):=\left[1-g\left(\frac{\vec{\xi}}{\theta}\right)\right]v(\vec{\xi}) \tag{130}$$

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

$$H:=H_0+\varepsilon v \tag{131}$$

and

$$H_1\equiv H_{1,\theta}:=H_0+\varepsilon w_\theta, \tag{132}$$

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

$$H=H_1+\varepsilon\,\delta v_\theta. \tag{133}$$

From standard texts on rigorous atomic physics (e.g., Kato, 1980; Cycon, Froese, Kirsch, and Simon, 1987) we know that the spectrum of $H_0$ consists of an infinity (for an attractive Coulomb potential) of eigenvalues,

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

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

$$E_{k_E+1}-E_{k_E}=:2d_E>0. \tag{134}$$

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

$$|\psi_j(\vec{\xi})|\leq c_{E,\delta}e^{-(\tilde{\mu}_E-\delta)|\vec{\xi}|}, \tag{135}$$

for any $\delta>0$, where $c_{E,\delta}$ is a finite constant; see, for example, Cycon, Froese, Kirsch, and Simon (1987). Thus eigenfunctions of $H_0$ decay *exponentially* at infinity. Given $\theta<\infty$, with $\theta\geq\theta_0$, we shall choose $\varepsilon$ so small that

$$\varepsilon\Lambda_\theta < \frac{d_E}{|E+k|}, \tag{136}$$

where $k$ is the constant appearing in Eq. (129). Thanks to Eqs. (129) and (136), 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 essentially the same as those developed in Application 1; see Eqs. (87)–(90). The projection operator $P_E$ is defined by

$$P_E = \frac{1}{2\pi i}\oint_{\gamma_E} dz\,(z-H_1)^{-1}, \tag{137}$$

where the contour $\gamma_E$ has been defined in Application 1 [cf. Eqs. (87)–(89)]. Furthermore, Eq. (90) 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 Eqs. (91) and (92), and show that

$$\int |\Pi_E(\vec{\xi},\vec{\eta})|^2 e^{2\alpha(|\vec{\xi}|+|\vec{\eta}|)} d^3\xi d^3\eta \leqslant (k_E C_E)^2, \tag{138}$$

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 (138) follows from (135), by the Combes-Thomas argument. Note that Eq. (138) claims exponential, rather than Gaussian (as in Application 1), decay of $|\Pi_E(\vec{\xi},\vec{\eta})|$, as $|\vec{\xi}|+|\vec{\eta}|\to\infty$.

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 $\rho_0$ with the property that, for some $\sigma<1$, there exists some $E<E_c$ such that

$$\mathrm{tr}(\rho_0 P_E) \geqslant (1-\sigma)^2. \tag{139}$$

We set $p_t := \mathrm{tr}(\rho_t P_E)$, $q_t := \mathrm{tr}(\rho_t Q_R)$, where $Q_R$ projects onto the subspace of Pauli spinors in $\mathscr{H}$ that vanish outside a sphere of radius $R$ centered at the origin of $\mathbb{R}^3$. Again, by Eq. (138), we have

$$\|(1-Q_R)P_E\| \to 0 \text{ as } R\to\infty; \tag{140}$$

see Eq. (106). The estimate replacing (101) now reads

$$0 \leqslant \mathrm{tr}(-[P_E,\delta v_\theta]^2) \leqslant 2\delta_E^2 e^{-2\mu_E\theta}, \tag{141}$$

for $\theta \leqslant \theta_0$ [see Eq. (130)] and $E<E_c$, where $\delta_E$ is a finite constant, and $\mu_E$ is positive. Recalling that $H=H_0+\varepsilon v$, we conclude that if $\varepsilon>0$ satisfies Eq. (136), and for $\sigma$ sufficiently small,

$$p_t \overset{\leqslant}{\geqslant} \sin_*^2\left(\frac{\pi}{2} - \sqrt{2^{\mp 1}\sigma} \pm t\varepsilon\,\delta_E e^{-\mu_E\theta}\right). \tag{142}$$

Assuming that $\rho_0$ is chosen such that

$$\mathrm{tr}(\rho_0 P_E) = 1 \text{ for some } E<E_c, \tag{143}$$

then one derives from Eqs. (142) (with $\sigma=0$) and (140) that, given any $\Delta>0$, there exists some $R_\Delta<\infty$ and a constant $\tau_{E,\Delta}>0$ such that if $\varepsilon$ satisfies Eq. (136) then

$$q_t \geqslant 1-\Delta, \tag{144}$$

for all $R\geqslant R_\Delta$ and $|t|\leqslant \varepsilon^{-1}\tau_{E,\Delta}e^{\mu_E\theta}$. Thus the escape time to infinity of the electron grows exponentially in $\theta$, where $\theta$ can be chosen so large that $\varepsilon\Lambda_\theta \leqslant$ const [see Eq. (136)].

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

$$v(\vec{\xi}) = \xi_1, \tag{145}$$

i.e., $\varepsilon v(\vec{\xi}) = \varepsilon\xi_1$. This is the Stark problem for a constant, external electric field $\vec{E}=(-\varepsilon/e,0,0)$ in the $x$ direction. Setting $k=-E_0+1$ in (129), we then have

$$\|w_\theta\psi\| \leqslant \theta\|\psi\| \leqslant \theta\|(H_0+k1)\psi\|, \tag{129'}$$

i.e., $\Lambda_\theta = \theta$. Hence, given $\varepsilon>0$ and taking into account Eq. (136), we may set

$$\theta = \kappa_E\varepsilon^{-1}, \tag{146}$$

for some constant $\kappa_E>0$. Then Eqs. (142) and (144) yield

$$p_t \overset{\leqslant}{\geqslant} \sin_*^2\left(\frac{\pi}{2} - \sqrt{2^{\mp 1}\sigma} \pm t\varepsilon\,\delta_E e^{-\nu_E\varepsilon^{-1}}\right), \tag{147}$$

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

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

Thus the escape time of the electron to $\infty$ is exponentially large in $1/\varepsilon$!

**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 Eqs. (123) and (125) we infer that if we set $\varepsilon = eqB_*^2/(Mc^2)$ then we may choose $\theta$ so large that

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

for some constant $\kappa_E>0$, where the term $\theta^2$ comes from the centrifugal potential $\xi_1^2+\xi_2^2$ in Eq. (125). Thus, as long as $r^2 \gg \kappa_E/\varepsilon$, $\theta$ grows like $1/\varepsilon$; but, asymptotically, as $\varepsilon\downarrow 0$, $\theta$ grows like $1/\sqrt{\varepsilon}$. Physically, $\varepsilon$ is very small, so that the escape time of the electron to infinity is comparatively very large.

We make the following remarks:

(1) The techniques developed in Application 2 can be generalized to yield lower bounds on lifetimes of states of multielectron ions in external electromagnetic fields.

(2) The methods developed in this paper can be applied to prove lower bounds on the lifetimes of excited states of atoms when the electrons are coupled to the quantized electromagnetic field. These bounds agree with those expected from perturbation theory (Bach, Fröhlich, and Sigal, 1995).

(3) The methods developed in this paper are efficient for proving lower bounds on the lifetimes of unstable states. More detailed estimates, including the term $f(\rho_0,\tilde{H}_s)$ in Eq. (54) and improved trial propagators, are required for obtaining upper bounds on lifetimes or for deriving a detailed, temporal picture of a decay process. Hunziker (1990), has constructed methods complementary to ours, based on the

technique of complex dilations, in order to describe the decay of unstable states and obtain bounds on lifetimes.

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