Two Time Localization

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Although quantum evolution equations are first order in time it is possible to define a state through partial information at multiple times. We consider the specification of position at two times and for a given Hamiltonian seek the wavefunction that minimizes the sum of the spreads at those times. We also study the time dependence of that minimal spread for a variety of Hamiltonians and boundary conditions.

1. INTRODUCTION

In classical mechanics one gives a pair of positions and times and seeks paths (any or many) that connect them. In quantum mechanics this is not the natural problem and what one usually prescribes is the wavefunction at a single time. Since quantum evolution equations are first order no further information can be given. In this article we offer a quantum analog of the two time boundary value problem in which the wavefunction is not the primary object specified, but is instead determined, as we describe below, from information at separated times.

Given two times $t_1$ and $t_2$ and two positions $x_1$ and $x_2$ (in $\mathbb{R}^n$), we seek a wavefunction that gives optimal localization about these events. The intervening time evolution is governed by a fixed, given Hamiltonian. Although our interest in this problem arises from certain physical questions [1] there is nevertheless freedom available in defining what is meant by "optimal." Since $\delta$-function localization at two times is generally impossible one is led to consider containment in a neighborhood of $x_i$ ($i = 1, 2$). Requiring that the wavefunction $\psi$ vanish identically outside two neighborhoods (at two respective times) also seems to us impossible so we weaken the concept of localization for our present purposes and go to what seems a more natural Hilbert space concept, namely a definition in terms of the spread of the wavefunction. For a given normalized wavefunction $f(x)$ and a given position $\bar{x}$ the square spread of $f$ is defined as

$$w(\bar{x}; f) = \int dx f^{*}(x)(x - \bar{x})^2 f(x)$$  \hspace{1cm} (1.1)

where $dx$ is an $n$-dimensional volume. For given $(x_i, t_i)$, $i = 1, 2$, we wish to
minimize the sum of the square spreads. To be precise, let \( H \) be the given Hamiltonian and \( \psi(x, 0) \) (or \( \psi_0 \)) the wavefunction at time 0. Then \( \psi(x, t_i), i = 1, 2, \) are the state vectors evolved from \( \psi_0 \) under \( H \), i.e.,

\[
\psi_{t_i} = e^{-iHt_i/h}\psi_0, \quad i = 1, 2. \tag{1.2}
\]

Let

\[
W(x_1, t_1, x_2, t_2; \psi_0) = w(x_1; \psi_{t_1}) + w(x_2; \psi_{t_2}); \tag{1.3}
\]

then we define our optimization problem to be the finding of \( \psi_0 \) such that \( W \) is minimized. Let

\[
\hat{x}(t) \equiv e^{iHt/h}\hat{x}e^{-iHt/h} \tag{1.4}
\]

be the Heisenberg picture position operator. Then \( W \) can be rewritten

\[
W(x_1, t_1, x_2, t_2; \psi_0) = \int dx \psi_0^* (x)[(\hat{x}(t_1) - x_1)^2 + (\hat{x}(t_2) - x_2)^2] \psi_0(x). \tag{1.5}
\]

From Eq. (1.5) it is clear that our problem is to find the smallest eigenvalue of the operator

\[
\hat{W}(x_1, t_1, x_2, t_2) = (\hat{x}(t_1) - x_1)^2 + (\hat{x}(t_2) - x_2)^2 \tag{1.6}
\]

(with appropriate rephrasing in case of a continuum spectrum).

In the next sections we explore solutions of this problem. We first treat the fully solvable quadratic Hamiltonians. Then in Section 3 we show that when the boundary conditions require nontrivial scattering additional spreading is forced on the system. In Section 4 we consider systems for which the classical boundary value problem allows a number of qualitatively different solutions and examine the way selection among these solutions can reduce the total two time spread. The last section is a summary and discussion.

2. Harmonic Oscillator and Free Particle

Let

\[
H = \frac{1}{2m} \hat{p}^2 + \frac{1}{2} m\omega^2 x^2. \tag{2.1}
\]

We consider all cases, \( \omega^2 \) positive, zero, and negative. Equation (1.4) can be integrated to yield

\[
\hat{x}(t) = \hat{x} \cos \omega t + \hat{p} \frac{\sin \omega t}{m\omega} \quad (\hat{p} = -i\hbar \hat{\nabla}) \tag{2.2}
\]
(which holds with appropriate limits or replacements for $\omega^2 = 0$ or $\omega^2 < 0$). The operator $\hat{W}$ can be written as a quadratic polynomial in $x$ and $p$ (dropping the circumflex) so that our problem's solution involves a second, derived harmonic oscillator Hamiltonian. It is convenient to make the transformation

\[ \xi = x - x_0, \quad \pi = p - p_0 \]  

with $x_0$ and $p_0$ the ("c-number") solutions to the equations

\[ x_i = x_0 \cos \omega t_i + p_0 \frac{\sin \omega t_i}{m\omega}, \quad i = 1, 2 \]  

(2.3)

(2.4)

(2.3)

(2.4)

(2.5)

Without loss of generality we take $t_1 = -T/2, t_2 = T/2$. $\hat{W}$ simplifies to

\[ \hat{W}(x_1, t_1, x_2, t_2) = \xi^2 (\cos^2 \omega t_1 + \cos^2 \omega t_2) + \pi^2 \left( \frac{\sin^2 \omega t_1}{m^2 \omega^2} + \frac{\sin^2 \omega t_2}{m^2 \omega^2} \right) \]

\[ + (\xi \pi + \pi \xi) \left( \frac{\cos \omega t_1 \sin \omega t_1}{m\omega} + \frac{\cos \omega t_2 \sin \omega t_2}{m\omega} \right). \]

(2.5)

Writing this as $\frac{1}{2} M^{-1} \pi^2 + \frac{1}{2} M \Omega^2 \xi^2$ we identify $\Omega$ as $2 |\sin \omega T| / m\omega$ and $\hat{W}$'s lowest eigenvalue is

\[ W_0 = \hbar |\sin \omega T| / m\omega. \]

(2.7)

This solves our problem for the quadratic Hamiltonian.

We study the solution for each case of interest.

1. Free particle. $\omega = 0$. $W_0 = \hbar T/m$ ($T > 0$). It follows that a particle's position can be specified at times separated by $T$ with a position uncertainty

\[ (\Delta x)_{\text{min}} = \frac{\sqrt{\hbar T}}{2m}. \]

(2.8)

This is the uncertainty at both $t_1$ and $t_2$ since the minimum is attained when the competing terms are equal. The growth with $T$ is a manifestation of inevitable wave packet spreading (in vacuum) and the square root shows this to be basically diffusive. A feature that may strike the reader as surprising is the fact that $(\Delta x)_{\text{min}}$ is independent of $|x_1 - x_2|$. Thus for $T = 0$ we would naturally expect $\Delta x = 0$ as long as $x_1 = x_2$: this is just the fact that we can localize a particle arbitrarily well at a single time as long as we are willing to pay the price in terms of high momentum.
components. But for \( x_1 \neq x_2 \) as \( T \downarrow 0 \) one might have thought that localization at finitely separated points would force momentum components that preclude small \( \Delta x \). The resolution of this paradox is that the transport from \( x_1 \) to \( x_2 \) is accomplished with a factor \( \exp(\pm i m (x_2 - x_1)/\hbar T) \), which corresponds to high momentum but not momentum spread (cf. Eq. (2.13) below). It is amusing to put numbers in Eq. (2.8). For \( m_H \) = hydrogen atom mass, (2.8) becomes in cgs units

\[
(\Delta x)_{\text{min}} = 1.78 \times 10^{-2} \frac{m_H}{m} \frac{\sqrt{T}}{\sqrt{\text{sec}}} \text{ cm.}
\]  

Thus a light atom located in vacuum for a few seconds must have a wavefunction spread on a scale of millimeters (at the beginning or end of its isolation, at least). However, several seconds of confinement in a vacuum chamber requires extremely low mean momentum (the spread in momentum is already taken into account in (2.8)).

II. Harmonic oscillator. \( \omega > 0 \). \( W_0 = \hbar |\sin \omega T|/m\omega \). Of interest in this case is the fact that \( W_0 \) vanishes periodically. For an initial \( \delta \)-function "wavefunction," localization is perfect. Although large momenta contribute to this state the harmonic potential focuses them perfectly at intervals of \( \pi/\omega \). The optimum wavefunction, that for which \( W = W_0 \), turns out to be a coherent state. Writing it as a function of \( x \) involves backtracking through our definitions. For \( \bar{W} \) of (2.6) the ground state wavefunction is

\[
\bar{\psi}(\xi) = (M\Omega/\hbar\pi)^{1/4} \exp(-M\Omega \xi^2/2\hbar)
\]  

with

\[
\Omega = 2 |\sin \omega T|/m\omega \]

\[
M = \frac{m^2 \omega^2}{4 \sin^2(\omega T/2)}.
\]

In terms of \( x \),

\[
\psi(x) = \left( (m\omega/\hbar\pi) \csc(\omega T/2) \right)^{1/4} \exp\left[ -m\omega \csc(\omega T/2)(x - x_0)^2/2\hbar + ip_0 x/\hbar \right] \]

with \( x_0 \) and \( p_0 \) given through (2.4). (The phase factor in (2.12) arises from the \( p \) translation in (2.3).) Note that for \( \omega T \to n\pi \) this does indeed approach a representation of the \( \delta \)-function. For the free particle \( \omega \to 0 \), \( x_0 = (x_1 + x_2)/2 \), \( p_0 = m(x_2 - x_1)/T \), and

\[
\psi(x) = \left( \frac{2m}{\pi\hbar T} \right)^{1/4} \exp\left[ -\frac{m}{\hbar T} (x - x_0)^2 + ip_0 x \right].
\]  

This provides the promised phase factor for overall transport from \( x_1 \) to \( x_2 \) (no matter how small \( T \)) and shows the optimum localization strategy \([2]\) to be
localization with position uncertainty \( \sqrt{\hbar T/4m} \) at \( t = 0 \) with spreading to \( \sqrt{2} \) times that at \( \pm T/2 \).

III. Inverted oscillator. \( \omega^2 = -\omega'^2 < 0 \). \( W_0 = \hbar \sinh \omega' T/m \omega' \ (T > 0) \). Wave packet spreading in this case is dramatic. The dominant effect is no longer diffusion; instead it is the fact that at larger \( |x| \), the driving force toward yet larger \( |x| \) grows. This is the simplest example of classical time evolution with positive Liapunov exponent: Paths with slightly different initial conditions diverge from each other exponentially. As we have seen, the quantum consequence of this property is extremely rapid wave packet spreading. Presumably similar behavior occurs in other cases such as spaces of negative curvature. There is a good deal of interest in the quantum consequences of unstable behavior at the classical level [3], this issue coming under the rubric "quantum chaos." The rapid, nondiffusive wave packet spreading is an immediate and uncomplicated result of the classical instability.

3. ONE DIMENSIONAL SCATTERING: LINEAR GROWTH OF \( \Delta x \)

Let \( H = p^2/2 + V(x) \), \( x \in \mathbb{R} \), and \( V(x) \) be a potential with support near the origin. In this section we take \( m = 1 \) and \( \hbar = 1 \). We demand localization at positions on opposite sides of the potential so that the particle is necessarily scattered at some stage in its progress. We concentrate on the case \( x_1 = vt_1, \ t_1 = -T/2, \ t_2 = T/2, \ v \) fixed, and \( T \) large. In particular we show that (generically) as \( T \to \infty \), \( \Delta x \) grows like \( T \), rather than \( \sqrt{T} \) as in the free particle case. What is happening is that once the particle strikes the potential the transmitted and reflected waves move away from each other with velocity \( v \). The mean position is somewhere between them but the spread grows linearly in \( T \). This is also true if some of the wavefunction is trapped in bound states near zero.

Our observation on the \( O(T) \) separation of the wave packets after scattering may seem so obvious that a section devoted to proving this point should be superfluous. The substantive part of our assertion is the claim that no matter what initial wave packet is selected, there always will be both a scattered and a reflected wave. One might have thought that with shrewd tailoring of the initial packet one could arrange for different pieces of, say, the reflected wave to interfere destructively so that pure transmission occurs (under circumstances in which an uncomplicated packet, such as a coherent state, would have nonzero reflection. Thus we exclude reflectionless potentials or special resonances.) What we will show is that a wave packet with reasonable initial localization cannot be so tailored [4].

Consider then a wave packet coming from the left. Sufficiently far into the past it has no overlap with the origin so that its form and time dependence are

\[
\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \, \phi(k) \exp \left( ikx - \frac{ik^2t}{2} \right), \quad t < 0, |t| \text{ large.} \tag{3.1}
\]

Our goal is to show that the sum of the past and future spreads \( \Delta x \) (\( = \sqrt{\langle \Delta x \rangle^2} \))
is at least of order $T$. To prove this we assume the contrary. That is $\psi(x, t)$ in (3.1) will be taken to have spread less than $T$. This assumption will be shown to constrain the spread in $k$. Narrowness in momentum space will then be used to show that the packet is scattered to both the left and the right. The scattered waves move apart linearly in $t$, implying the same growth for $\Delta x$, contrary to our original hypothesis.

From (3.1) it follows that

$$\bar{x} \equiv \langle x \rangle = \int dx \psi^*(x, t) x \psi(x, t) = vt + x_0 \quad (3.2)$$

with

$$\phi = \rho e^{i\theta}, \quad \rho, \theta \text{ real} \quad (3.3)$$

$$v = \bar{k} = \langle k \rangle = \int dk \rho^2 k \quad (3.4)$$

$$x_0 = \int dk \phi^* i \frac{\partial}{\partial k} \phi = -\langle \frac{d\theta}{dk} \rangle. \quad (3.5)$$

Higher moments are derived using

$$(x - \bar{x})^n \psi(x, t) = \frac{1}{\sqrt{2\pi}} \int dk e^{ik(x - \bar{x})} \left(i \frac{\partial}{\partial k}\right)^n (\phi e^{ik\bar{x} - ik^2/2}) \quad (3.6)$$

It follows that

$$\langle (x - \bar{x})^n \rangle = \int dk \Phi^* \left(i \frac{\partial}{\partial k}\right)^n \Phi \quad (3.7)$$

with $\Phi = \phi(k) e^{ik\bar{x} - ik^2/2}$. Strictly speaking, to establish results analogous to those in Section 2, we should deal only with $\langle (x - \bar{x})^2 \rangle$. In the present section however we interpret the limitation on the spread differently and assume that for $t \to -\infty$, for each $n$,

$$\frac{\langle (x - \bar{x})^n \rangle}{t} \to 0 \quad \text{as} \quad |t| \to \infty \quad (t < 0). \quad (3.8)$$

From (3.7) it follows that the highest power of $t$ in $\langle (x - \bar{x})^n \rangle$ is obtained by differentiating the factor $\exp(ik\bar{x} - ik^2t/2)$ $n$ times. Thus

$$\langle (x - \bar{x})^n \rangle = \langle (k - \bar{k})^n \rangle t^n + O(t^{n-1}). \quad (3.9)$$

To satisfy (3.8) we must have $\langle (k - \bar{k})^n \rangle \to 0$ as $|t| \to \infty$, for all $n$. (A word of explanation may be in order here since $\phi$, and moments computed with $\phi$, have no explicit time dependence. Recall that we have been given $v$ and $T$ and are seeking
that \( \phi \) which minimizes \( W \). For fixed \( v \), as \( T \) is increased the optimizing \( \phi \) will change and so will moments computed with it. Our assumption, which we ultimately plan to contradict, is that \( \phi \) can be selected so that \( \Delta x = o(|T|) \) for both negative and positive \( T \). Using (3.9) this in turn implies all \( k \)-space moments go to zero. That will in turn imply nontrivial scattering and yield the desired contradiction.)

Having established properties of \( \phi(k) \) from spatial properties of the wavefunction in the distant past, we next turn to the wavefunction after the scattering by \( V(x) \). For \(|x| > |\) greater than the support of \( V \) the wave function is

\[
\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \ A(k) \phi(k) \exp\left(-ikx + \frac{ik^2t}{2}\right), \quad x < 0, \quad t \to +\infty \quad (3.10a)
\]

\[
\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \ B(k) \phi(k) \exp\left(ikx - \frac{ik^2t}{2}\right), \quad x > 0, \quad t \to +\infty. \quad (3.10b)
\]

The functions \( A \) and \( B \) are the scattering matrix for this one-dimensional problem. They can be written \( A = ae^{ix}, \ B = be^{-ix}, \) with \( a, b, x, \) and \( \beta \) real and \( a^2 + b^2 = 1. \) The form (3.10) is valid under conditions more general than those ordinarily considered in scattering theory. In the usual scattering theory \([S, 61,\) in order to connect time independent continuum solutions to cross sections used for wave packets one demands \( \langle (k - \bar{k})^2 \rangle \leq m/2\hbar T. \) This prevents wave packet spreading during the course of the experiment. That condition is more stringent than our demand on the second moment. We allow this generality because we wish to prove that even with more leeway in \( k \)-space it will still be impossible to construct packets that are perfectly reflected or perfectly transmitted. To see what is required for the validity of (3.10) recall that (3.10) is based on the following continuum solution of the static problem,

\[
u(x) = \begin{cases} 
e^{ikx} + A e^{-ikx}, & x < \text{min supp } V \\ B e^{ikx}, & x > \text{max supp } V. \end{cases} \quad (3.11)
\]

Thus for (3.10) to hold it is required in particular that the wave packet (3.1) vanish for \( t \to +\infty \) and negative \( x \). To show this we use a stationary phase approximation for (3.1), based on the largeness of \( t \):

\[
\frac{\partial}{\partial k} \left( \theta(k) + kx - \frac{1}{2} k^2 t \right) = 0. \quad (3.12)
\]

Because of our restrictions on the moments of \( k, \) \( \phi \) will be small away from \( \bar{k}. \) Therefore unless \( \theta' \) is singular near \( \bar{k}, \) Eq. (3.12) requires that \( x = \bar{k}t \) and in particular that \( x \) be positive in order to have an integral of any size (failure to satisfy the stationary phase condition costs powers of \( 1/t). \) However, the requirement that for \( t \to -\infty \) the wave packet be centered on the large negative value \( x_1 \) precludes large \( \theta' \) at \( \bar{k}. \) Compare Eqs. (3.2) and (3.5). Therefore the packet
(3.1) does not contribute for large positive times. With appropriate smoothness conditions for \( a(k) \) and \( \beta(k) \) similar considerations apply to the scattered waves (3.10) causing them to vanish for \( t \rightarrow -\infty \). We have thus justified the use of (3.10), despite relaxation of the condition \( \langle (\Delta k^2) \rangle \leq 1/T \) (again taking \( h = m = 1 \)).

By stationary phase arguments the same as those used for (3.1) it follows that for \( t \rightarrow -\infty \) the wave packets are centered on \( \pm vt + O(1) \) where the \( O(1) \) corrections arise from \( \partial a/\partial k \), \( \partial \beta/\partial k \), and \( \partial A/\partial k \). Therefore, since \( x_2 = vT/2 > 0 \), to establish our basic claim that \( Ax \sim T \) it remains only to show that the norm of \( \psi \) on the left of the origin is bounded away from zero as \( t \rightarrow -\infty \). This will contradict our earlier assumption and establish that for scattering minimal wave packet spreading exceeds the diffusive lower bound. We must therefore show that for the function

\[
\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \ A(k) \phi(k) \exp \left( -ikx - \frac{ik^2t}{2} \right) \tag{3.10a}
\]

the square integral on the negative \( x \) axis is order unity. Consider

\[
J = \int_{-\infty}^{0} dx |\psi(x, t)|^2, \quad t \rightarrow +\infty. \tag{3.13}
\]

By our stationary phase arguments, \( \psi \) of (3.10a) will vanish with \( 1/t \) for \( x > 0 \), so that we extend the integral in \( x \) to \( +\infty \). It follows that

\[
J = \int_{-\infty}^{\infty} dk a^2(k) \rho^2(k). \tag{3.14}
\]

Expand (the smooth function) \( a(k) \) about \( \bar{k} = v \) to give

\[
J = \int_{-\infty}^{\infty} dk \rho^2(k) \left[ a(\bar{k}) + (k - \bar{k}) a'(\bar{k}) + \frac{1}{2}(k - \bar{k})^2 a''(\bar{k}) + \cdots \right]^2. \tag{3.15}
\]

The leading term is \( |a(\bar{k})|^2 \) and by our assumptions on \( a(k) \) this term is of order unity. It remains only to show that the other terms are of smaller order and therefore unable to cancel the leading term. The next nonzero term is

\[
\int dk \rho^2(k) \left[ (a'(\bar{k}))^2 + a(\bar{k}) a''(\bar{k}) \right](k - \bar{k})^2 = (\text{const}) \langle (k - \bar{k})^2 \rangle. \tag{3.16}
\]

Again our assumptions on \( a(k) \) deprive the constant of disruptive potential. The vanishing of \( \langle (k - \bar{k})^2 \rangle \) was found earlier to be required for the putative \( o(T) \) localization of \( \psi \) at negative times. Therefore for \( t \rightarrow +\infty \) the quantity in (3.16) vanishes. The same is true for the remaining terms in the expansion of (3.15) by virtue of our argument following (3.9).

This completes our demonstration. It falls short of rigor because of the smoothness assumptions on \( \phi \) that were needed for the stationary phase arguments.
We do not present complete information on optimizing functions—as appeared in Section 2—because the time dependent position operator \( \dot{x}(t) \) is not easy to represent. (Even for the \( \delta \)-function potential, for which an explicit time dependent Green's function is known [7, 8], the nonlocal terms in \( \dot{x}(t) \) preclude convenient manipulation.)

4. MINIMIZATION STRATEGIES

Consider two time localization for an \( N \) particle system where both \( N \) and \( T \) (the time between localizations) are large. We have in mind particles with realistic interactions such as the Lennard–Jones potential. The dynamical richness of this situation adds possibilities for the minimization of the spreading function

\[
W(\{\tilde{x}_{z,i}, t_x\}, \psi_0) = \sum_{x} \sum_{i=1}^{N} \int d^N x_i \psi_0^*(\dot{x}_i(t_x) - \tilde{x}_{z,i})^2 \psi_0,
\]

where \( z \in \{\text{initial, final} \} \), \( \{\tilde{x}_{z,i}\} \) are the boundary conditions, \( \dot{x}_i(t) \) are the Heisenberg position operators, and \( \psi_0 \) is the time zero \( N \)-body wavefunction.

We first suggest a minimization strategy for \( W \). The strategy depends on the existence of classical trajectories that satisfy or nearly satisfy the given boundary conditions and that allow the particles to be close to one another for much of the time interval. We do not know how broad the class of boundary conditions is for which such trajectories exist, although at the end of this section we suggest that with chaotic dynamics that class is large.

The general idea of the strategy is this. The \( N \) particles attract each other when brought moderately close but when far apart they do not interact. If they are widely separated throughout the time interval, the minimum of \( W \) is \( NT/\hbar/m \) (taking them all to have the same mass \( m \)). By contrast, if for most of the time they are in a few clumps, wave packet spreading is far smaller—most degrees of freedom are in approximate oscillator wells where the spread does not grow in time (cf. Eq. (2.7)). Let the interparticle oscillator frequency be \( \omega \). We show in Appendix A that the minimum value of \( W \) when the particles are bound in a harmonic chain is either \( \hbar T/m \) (if \( \omega T \gg N \)) or \( 2N\hbar/(\omega m) \log \omega T \) (if \( N \gg \omega T \)); in both situations the spreading is far smaller than \( NT/\hbar/m \).

If this strategy can work there will exist boundary conditions (widely separated) for which a wavefunction can be found to bring the particles into several clumps, remain that way for most of \( T \), and then break up toward the end of the period so as to meet their final conditions. At least part of this sequence would look like a billiards break run backward. Since we cannot actually exhibit such boundary conditions for the \( N \)-particle case we will offer two examples where successful minimization strategies are possible through selection among classical trajectories satisfying given boundary conditions. Following that we discuss the relevance of these examples to the \( N \)-particle scenerio.
Example I: Flat Bottomed Oscillator

Let \( x \in \mathbb{R} \) and

\[
H = \frac{p^2}{2m} + \theta(x - \frac{L}{2}) \frac{1}{2} m \omega^2 x^2 + \theta(-x - L) \frac{1}{2} m \omega^2 (x + L)^2.
\] (4.2)

Let \( \hat{x}_x = -L/2, \ x \) initial, final, and let \( L^2 \gg \hbar T/m. \) This problem allows two very different minimization strategies. One option is to stay near \( x = -L/2 \) the whole time; the wavefunction would be given by (2.13) with \( p_0 = 0. \) In this case \( W = \hbar T/m. \)

The second option is described semiclassically as follows: Use a spatially compact wave packet with extremely high initial mean velocity, say to the right. The packet quickly reaches \( x = 0. \) There it enters the oscillator potential, moves further right, is slowed down, and is sent back to 0 in time \( \pi/\omega. \) That time is independent of velocity. Moreover, since the packet spent exactly one-half period in the oscillator its wavefunction is as spread or unspread as when it entered. It now proceeds rapidly to the left where the same thing happens at \( -L. \) With sufficiently high velocity the time spent in the flat bottom region \( -L < x < 0 \) can be made arbitrarily small. On the other hand, the time spent with \( x < -L \) or \( x > 0 \) leads to no spreading. With a little fine tuning the mean position of the particles can be arranged to be \( -L/2 \) at the end of the time period. Thus the spread can be made arbitrarily small.

We now justify the foregoing assertions by detailed calculation. One could consider stationary states of the entire potential, but the largeness of \( L \) allows us to treat each impact of the packet on the harmonic oscillator wall as a separate scattering event. There are two points to establish: (1) A high momentum wave packet striking a harmonic wall is returned a time \( \pi/\omega \) later with size and shape unchanged. (2) In the course of each such scattering some amplitude is lost from the packet due to the discontinuity in \( V''. \) This must be shown to be negligible.

We consider scattering off the right hand wall \( V(x) = \theta(x) \frac{1}{2} m \omega^2 x^2 \) and study a wave packet coming from the left. The stationary states are

\[
u_k(x) = e^{ikx} + e^{-ikx + i\phi(k)}.
\] (4.3)

As indicated, we view this as a scattering problem, ignoring the wall a distance \( L \) to the left. The wavefunction for early times is given by

\[
\psi(x, t) = \int dk \exp(i k x - i k^2 t/2m) \tilde{\psi}(k).
\] (4.4)

\( \tilde{\psi}(k) \) is assumed to be sharply peaked about some \( \bar{k} \) and for convenience in locating the particle we take \( \partial \tilde{\psi}/\partial \bar{k} = 0. \) Stationary phase arguments give the position where \( \psi(x, t) \) is largest to be

\[
x = h \bar{k} t/m, \quad t \to -\infty.
\] (4.5)
By the same arguments, for large positive times

\[ x = -\hbar \dot{t}/m + \phi'(k), \quad t \to +\infty. \quad (4.6) \]

(The "infinity" for \( t \) is of course far less than \( T \).) A straightforward calculation gives

\[ \tan \frac{1}{2} \phi(k) = \sqrt{\frac{2}{v + (1/2)}} \frac{\Gamma(v/2 + 1)}{\Gamma(v/2 + 1/2)} \tan \frac{\pi v}{2}, \quad (4.7) \]

where

\[ v = \frac{E}{\hbar \omega} \left( \frac{1}{2} \right), \quad E = \frac{\hbar^2 k^2}{2m}. \quad (4.8) \]

For large \( v \), Stirling's formula applied to (4.7) yields

\[ \tan \frac{1}{2} \phi \simeq \sqrt{\frac{v + 1}{v + 1/2}} \tan \frac{\pi v}{2} \simeq \left( 1 + \frac{1}{4v} \right) \tan \frac{\pi v}{2}. \quad (4.9) \]

From (4.9) it is seen that \( \partial \phi/\partial v \) is close to \( \pi \) (the difference drops off at least as fast as \( \pi/4v \)) so that

\[ \frac{\partial \phi}{\partial k} = \frac{\partial \phi}{\partial v} \frac{\partial v}{\partial k} = \frac{\pi \hbar k}{\omega m}. \quad (4.10) \]

Substituting (4.10) in (4.6) we find precisely the delay \( \pi/\omega \). The near linearity of \( \phi \) as a function of \( v \) reflects the harmonicity.

How significant is the deviation from perfect harmonic behavior? In the stationary phase context of (4.6) the deviation leads to a slight distorting of the wave. A similar but potentially more serious problem arises from this same deviation. This is the possibility that some scattering takes place as the packet first enters the potential, a region where \( V'' \) is discontinuous. An effect analogous to above-barrier-scattering \([9]\) will occur.

To estimate this effect we consider the value of \( \psi \) at positive times and at points \( x \) such that \( x_R = -\hbar \dot{t}/m \), since this would be the position of that piece of the packet that is reflected as the packet crosses \( x = 0 \). At such \( x_R \), the argument of the exponent in the integral over \( k \),

\[ \psi(x_R, t) = \int dk \exp(ikx_R - i\hbar k^2 t/2m + i\phi) \psi(k), \quad (4.11) \]

is not stationary. To calculate how large \( \psi(x_R, t) \) is we distort the contour of \( k \) integration to find a complex \( k \) value where \( \phi' = 0 \). Having found this, \( \exp(i\phi) \) evaluated at the complex \( k \) will no longer be of norm one and \( |\exp(i\phi)|^2 \) is the probability of scattering at the discontinuity in \( V'' \).

We seek therefore simultaneous solution of (4.7) and \( \partial \phi/\partial v = 0 \). The
approximations leading to (4.9) are true for complex $v$ as long as $|v|$ is large and $\arg v < \pi$. It follows that $v$ must satisfy

$$v^2 \left( 1 + \frac{1}{4v} \right) = \frac{1}{4\pi} \sin v\pi$$

which has the approximate solution

$$\text{Im } v \sim \text{const} + \frac{2}{\pi} \log \text{Re } v, \quad \text{Re } v \sim \text{integer} + \frac{1}{2}.$$  \hspace{1cm} (4.12)

For such $v$ we have

$$|e^{i\phi}| \sim \frac{1}{8\pi |v|^2}. \hspace{1cm} (4.14)$$

After $M$ scatterings the amplitude surviving in the original wave packet is $(1 - 1/8\pi |v|^2)^M$. In this case, $M \sim \omega T/\pi$, which is large. However, there is no limit on the size of $v$, so that by increasing $v$ the wave packet spreading can be held as small as desired.

This example shows that minimization strategies are possible. The unrealistic potential deprives the example of direct physical relevance.

**Example II: Conspiratorial Scattering**

Initial and final mean positions are given for four particles A, B, C, and D. At large distances they do not interact and the boundary conditions do not force them together. Thus we have the usual spreading bound, $\hbar T(m_A^{-1} + m_B^{-1} + m_C^{-1} + m_D^{-1})$. We now show that with the right boundary conditions and interparticle forces there is available a strategy of the sort contemplated for our $N$-particle system. Moreover, like that strategy, an observer watching the unfolding events would consider them to be unlikely (in the sense of random initial conditions).

Let A and B interact with a short range harmonic oscillator–like potential (with angular frequency $\omega$) but with long range indifference. Let the A–C, A–D, and C–D interactions be infinite hard core repulsion and nothing else. Let all other interparticle forces vanish. Take $m_C = m_D < m_A$. Take $m_B \ll m_C$ so most spreading is due to B. We work in one dimension. Our scheme is illustrated in Fig. 1. Initially A, C, and D all move toward B. A and C meet there with precisely the right velocity relation to bring A to a halt. A and B now remain together and their wave packet spreading is limited. C goes off to the right where it meets D whose velocity is tailored to send C back to the orbiting A–B pair. A–B is split and all particles go to their final positions. For appropriate boundary conditions, velocities will exist to make this scenario a solution to the equation of motion.

The quantum behavior follows the classical description provided that the kinetic energies are much larger than the A–B well depth.
Because Example II uses nongeneric boundary conditions it does not address the question of how often for the \( N \)-particle system there will be paths satisfying the boundary conditions that also manage to minimize wavefunction spreading. (But it does illustrate the point that successful minimization strategies will appear "unlikely.") We expect that for many particle systems with realistic dynamics the number of trajectories nearly satisfying given positional boundary conditions will be large and that among them will be found trajectories that minimize spreading as well. The reason for believing that number to be large is as follows [10]: Imagine chaotic motion (positive Liapunov exponent \( \lambda \)) on a compact \( n \)-dimensional space of volume \( V \). Give boundary conditions \( x(0) \) and \( x(2T) \) with \( \lambda T \gg 1 \) and allow an error \( \varepsilon \) in meeting those boundary conditions. We will show that for many values of \( x(T) \) it is possible to satisfy the 0 and \( 2T \) boundary conditions. Pick \( x(T) \) and vary \( \dot{x}(T) \). Because of the instability there will be many values of \( \dot{x}(T) \) that cause \( x(\cdot) \) to satisfy one or the other of its boundary conditions; in fact the successful values will form islands with narrow dimension \( \varepsilon \exp(-\lambda T) \) but with aggregate volume \( \varepsilon^n/V \). Again because of the instability (the system loses all memory on this time scale), there is no reason for these islands not to overlap; therefore a fraction \( (\varepsilon^n/V)^2 \) of \( \dot{x}(T) \) values will satisfy both boundary conditions. In this way the instability of the motion allows the (approximate) satisfaction of boundary conditions that parameter counting alone would seem to preclude [11].

5. DISCUSSION

In this article the two time localization problem has been defined to be the specification of two positions at two given times and the finding of a wavefunction that minimizes the sum of the (square) position spreads about those points at those times. For quadratic Hamiltonians a full solution of this problem was found. In particular we examined the growth of the minimal spread as a function of the time separation \( T \). For the free particle the growth was diffusive, \( \Delta x \sim \sqrt{T} \). In a har-
monic oscillator an oscillating spread was found so that perfect localization can be achieved at more than one time. For an inverted oscillator the minimal spread was found to grow exponentially in $T$. For more complicated Hamiltonians explicit solutions were not presented. However, for a scattering situation (times $\pm T/2$, positions $\pm vT/2$, $v$ given, support of $V$ near the origin) arguments were given for the minimal spread growing linearly in $T$; there is no way to tailor a wavefunction for perfect transmission or reflection. (We are not considering special situations, such as reflectionless potentials, where unusual potentials or resonances might allow this.)

In the section on minimization strategies the results of the earlier sections were used to approach a more difficult problem: Given a large and widely distributed collection of particles with realistic interactions, is it possible for them to be well localized both in the remote past and future? We found that wave packet spreading could be substantially reduced provided that there existed certain classical trajectories. Arguments in favor of the existence of such trajectories were offered.

Other definitions of the two time localization problem are possible. For example, one could seek to minimize the product $(\Delta x)_1 (\Delta x)_2$. (In our earlier notation this would be $[w(x_1, \psi_{\chi_1}) \cdot w(x_2, \psi_{\chi_2})]^{1/2}$.) A lower bound for the product is gotten by an easy generalization of the uncertainty principle. For Hermitian operators $A$ and $B$, suppose $[A, B] = iC$. Then by the Schwartz inequality

$$\langle (A - \langle A \rangle)^2 \rangle \langle (B - \langle B \rangle)^2 \rangle \geq \frac{1}{4} \langle C \rangle^2.$$  \hspace{1cm} (5.1)

For quadratic Hamiltonians one again has a solvable problem and building $A$ and $B$ appropriately from $\dot{x}(t)$, etc., one obtains

$$(\Delta x)_1 (\Delta x)_2 \geq \frac{\hbar}{2m} \frac{\sin \omega T}{\omega}.$$  \hspace{1cm} (5.2)

For a free particle the product is therefore bounded from below by $\hbar T/2m$ [12]. This result could be used to obtain Eq. (2.7) as a consequence of the inequality between arithmetic and geometric means. Our preference for the sum formulation arises from the expectation that for the general case it is easier to work with. In fact that same inequality of means indicates that statements about the product are more stringent. Thus, for example, the kind of result established in Section 3 would be more difficult to obtain (if it is true) for products than for sums. Also, in a many particle context it would not be clear how to generalize the product formulation. Nevertheless, at the formal level of our investigation, the choice is a matter of taste.

As indicated above our interest in this problem was stimulated by issues associated with quantum measurement theory, and we hope at a later time to employ the bounds given here to those considerations. The inequality (5.2) has already been used in connection with a proposed [13] experiment that would distinguish between the Copenhagen interpretation and that proposed in Ref. [1].

Our emphasis in this article has been on defining the two time boundary value
problem in quantum mechanics. However, many of the features of our solutions have been observed in studies of the semiclassical evolution of wave packets in the usual context of an initial value problem. For example, Ref. [143] discusses systems whose spread is periodic in time and chaotic systems in which distributions spread exponentially. There are two reasons for these parallels. First, for the simple cases where we managed to find explicit solutions (Section 2) the optimizing functions are just the sort of packets best treated by semiclassical methods. In addition, in our Section 4 extensive appeal was made to semiclassical methods and use was made of the results of Section 2 with their corresponding semiclassical flavor (although in Section 2 all results are exact). It should be noted however that the calculation of Section 3 showing $O(T)$ spreading for nontrivial scattering is fundamentally not semiclassical. I say this despite the use of stationary phase methods in the asymptotic ($|T| \to \infty$) regime and despite the possibility that for each $V(x)$ of finite support one might invent a “geometrical theory of diffraction” to describe the scattering. This is because the scattering functions $A(k)$ and $B(k)$ are arbitrary and the existence or nonexistence of packets in the asymptotic regime does not depend on $\hbar$. The size of $\hbar$ only fixes the scale of $T$ required for those asymptotics to hold.

APPENDIX A: WAVE PACKET SPREADING FOR A CHAIN OF OSCILLATORS

We calculate the minimal spread of a (closed) chain of particles coupled by nearest neighbor attractive forces well approximated as pairwise oscillators with angular frequency $\omega$. The normal mode frequencies are then

$$\omega_j = 2\omega \sin \theta_j, \quad \theta_j = j\pi/N, \quad j = 0, 1, \ldots, N/2$$

(A.1)

(with nonzero modes counted twice). By (4.1) and (2.7) the minimal spread is

$$W_0 = \frac{\hbar}{m} \sum_{j=-N/2}^{N/2} \frac{|\sin(2\omega T \sin \theta_j)|}{2\omega |\sin \theta_j|}.$$  \hspace{1cm} (A.2)

We distinguish two cases, (I) $\omega T \gg N$ and (II) $N \gg \omega T$. In the first case separate the $j=0$ term and write

$$W_1 = \frac{\hbar T}{m} + \frac{2\hbar}{m} \sum_{j=1}^{N/2} \frac{|\sin(2\omega T \sin (j\pi/N))|}{2\omega \sin (j\pi/N)}.$$  \hspace{1cm} (A.3)

Since $\omega T \gg N$, for successive terms in the sum the quantity $|\sin(2\omega T \sin (j\pi/N))|$ will change considerably and this factor is replaced by $\langle |\sin \theta| \rangle$, namely $2/\pi$. Therefore

$$W_1 = \frac{\hbar T}{m} + \frac{2\hbar}{m \omega \pi \cdot \frac{\pi}{2N}} \left( N \int_0^{\pi/2} \frac{\sin \theta}{\sin \theta} \right) \frac{1}{\sin \theta}.$$  \hspace{1cm} (A.4)
Performing the integral we get

\[ W_1 = \frac{\hbar T}{m} + \frac{2\hbar}{m} \frac{1}{\omega n^2} N \log N. \]  

Whether or not the second term is important (i.e., even if \( N \log N > \omega T \)), \( W_1 \) is far less than \( \hbar N T/m \), the spread one would obtain if the \( N \) particles were separated and noninteracting. If \( N \log N \ll \omega T \) (as well as \( N \ll \omega T \)) it is seen that \( W_1 \) is dominated by the center of mass contribution \( \hbar T/m \). Note that this is \( N \) times the spread in the center of mass wavefunction \( (= \hbar T/(Nm)) \) since that spreading contributes \( N \) times when (4.1) is written in normal coordinates.

For Case II, \( N \gg \omega T \), \( W_0 \) can be written entirely as a continuum integral

\[ W_n = \frac{\hbar}{\omega m} \int_{0}^{\pi/2} \left( \frac{N}{\pi} \right) \left| \frac{\sin(2\omega T \sin \theta)}{\sin \theta} \right| d\theta. \]  

The integral

\[ J(u) = \int_{0}^{\pi/2} d\theta \left| \frac{\sin(u \sin \theta)}{\sin \theta} \right| \]  

behaves (for large \( u \)) like

\[ J(u) \sim \frac{2}{\pi} \log u. \]  

This can be seen by breaking the integration into ranges \( 0 \leq \theta \leq \pi/2R \) \( (J_1) \) and \( \pi/2R \leq \theta \leq \pi/2 \) \( (J_2) \) for some large fixed \( R \). The second integral is \( O(1) \) with a bound independent of \( u \). The first integral is rewritten

\[ J_1 = \int_{0}^{\pi/2R} dx \frac{\sin x}{x} \frac{1}{\sqrt{1 - x^2/u^2}} \]  

and is approximated by

\[ J_1 \sim \langle \sin x \rangle \int_{1}^{\pi/2R} dx \frac{2}{x} \sim \frac{1}{\pi} \log u. \]  

It follows that

\[ W_n \sim \frac{2\hbar N}{\omega m} \frac{1}{\pi^2} \log \omega T. \]  

In this case the spreading is mainly due to low frequency normal modes.
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REFERENCES

2. The wavefunction (2.13) as well as the Hamiltonian (2.6) for the \( \omega = 0 \) case have appeared in recent publications dealing with multiple time measurements. The issue in those articles is the connections of the quantum formalism with real physical measurement apparatus. The problem we define is formal. Therefore, although the class of Hamiltonians for which we solve our problem is wider than that of the indicated articles, without further interpretive steps our results do not bear on the measurement problems considered by those authors. Some of the literature is H. P. Yuen, Phys. Rev. Lett. 51 (1983), 719; C. C. Caves, Phys. Rev. Lett. 54 (1985), 2465; M. H. Partovi and R. Blankenbecler, Phys. Rev. Lett. 57 (1986), 2887, 2891.
4. For a slightly different formulation the \( O(T) \) behavior is not obtained. Specifically if \( x_1 \) and \( x_2 \) are held fixed and \( T \to \infty \) one gets \( \sqrt{T} \) behavior. This is because for sufficiently large \( T \) the spreading encompasses both \( x_1, x_2 \) and the support of \( V \). Thus the condition \( x_i = 0, t, |t| \to \infty \), is essential.
11. Our discussion ignores constants of the motion as well as the possibility that the collective behavior of the system may have strange attractors. In the latter case, if \( x(0) \) and \( x(2T) \) are far from the attractor the chance of reaching them from a time \( T \) position, presumably near the attractor, is less than \( e^{-T/V} \). If the system with attractor is microscopically Hamiltonian and time reversal invariant, which we take it to be, there will in principle be paths away from the attractor albeit of relatively small measure. As before, the loss of memory due to the instability suggests that escaping from the attractor at both times will introduce nothing worse than the square of that small number. Whether that quantity is unreasonably small will depend on the allowed tolerance \( \varepsilon \). A matter we have not confronted is whether the precision required in these classical specifications can be reflected in the quantum wavefunction. As a general comment on this question we mention the remarkable efficacy of semiclassical methods applied to classically ergodic systems. See the article by Gutzwiller referenced above [3] and a forthcoming book by that author.