Simple examples of position-momentum correlated Gaussian free-particle wavepackets in one-dimension with the general form of the time-dependent spread in position

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(Dated: February 1, 2008)
Abstract

We provide simple examples of closed-form Gaussian wavepacket solutions of the free-particle Schrödinger equation in one dimension which exhibit the most general form of the time-dependent spread in position, namely \( (\Delta x_t)^2 = (\Delta x_0)^2 + At + (\Delta p_0)^2 t^2 / m^2 \), where \( A \equiv \langle (\hat{x} - \langle \hat{x} \rangle_0)(\hat{p} - \langle \hat{p} \rangle_0) + (\hat{p} - \langle \hat{p} \rangle_0)(\hat{x} - \langle \hat{x} \rangle_0) \rangle_0 \) contains information on the position-momentum correlation structure of the initial wave packet. We exhibit straightforward examples corresponding to squeezed states, as well as quasi-classical cases, for which \( A < 0 \) so that the position spread can (at least initially) decrease in time because of such correlations. We discuss how the initial correlations in these examples can be dynamically generated (at least conceptually) in various bound state systems. Finally, we focus on providing different ways of visualizing the \( x - p \) correlations present in these cases, including the time-dependent distribution of kinetic energy and the use of the Wigner quasi-probability distribution. We discuss similar results, both for the time-dependent \( \Delta x_t \) and special correlated solutions, for the case of a particle subject to a uniform force.

Keywords: wave packets, time-development, correlations, Gaussian

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I. INTRODUCTION

The study of time-dependent solutions of the one-dimensional Schrödinger equation is a frequent topic in many undergraduate textbooks on quantum mechanics. The problem of a Gaussian or minimum-uncertainty wavepacket solution for the case of a free particle (defined more specifically below) is the most typical example cited, often being worked out in detail, or at least explored in problems \[1\]. The emphasis is often on the time-dependent position spread for such solutions, typically written in the forms

\[
(\Delta x_t)^2 = (\Delta x_0)^2 \left(1 + \left(\frac{t}{t_0}\right)^2\right) = (\Delta x_0)^2 + \frac{(\Delta p_0)^2 t^2}{m^2} \tag{1}
\]

where the spreading time or coherence time can be defined by \(t_0 \equiv m\Delta x_0/\Delta p_0\). Textbooks rightly point out the essentially classical nature of much of this result, explained by the fact that the higher momentum components of the wave packet outpace the slower ones, giving a position-spread which eventually increases linearly with time as \(\Delta x_t \approx \Delta v_0 t\), where \(\Delta v_0\) is identified with \(\Delta p_0/m\).

The form of the expression for \(\Delta x_t\) in Eqn. (1) is a special case of the most general possible form of the time-dependent spatial width of a one-dimensional wave packet solution of the free-particle Schrödinger equation which is well-known in the pedagogical literature \[2\] - \[9\], but seemingly found in many fewer textbooks \[10\]. This general case can be written in the form

\[
(\Delta x_t)^2 = (\Delta x_0)^2 + \langle(\hat{x} - \langle\hat{x}\rangle_0)(\hat{p} - \langle\hat{p}\rangle_0) + (\hat{p} - \langle\hat{p}\rangle_0)(\hat{x} - \langle\hat{x}\rangle_0)\rangle_0 \frac{t}{m} + \frac{(\Delta p_0)^2 t^2}{m^2} \tag{2}
\]

where the coefficient of the term linear in \(t\) measures a non-trivial correlation between the momentum- and position-dependence of the initial wave packet. While such correlations are initially not present in the standard Gaussian wave packet example routinely used in textbook analyses, which therefore gives rise to the simpler form in Eqn. (1), a non-vanishing \(x-p\) correlation does develop for later times as has been discussed in at least one well-known text \[11\] and several pedagogical articles \[12\].

For wave packets which are constructed in such a way that large momentum components \((p > \langle\hat{p}\rangle_0)\) are initially preferentially located in the ‘back’ of the packet \((x < \langle\hat{x}\rangle_0)\), the initial correlation can, in fact, be negative leading to time-dependent wave packets which initially shrink in size, while the long-time behavior of any 1D free particle wave packet is indeed
always dominated by the quadratic term in Eqn. \( \text{(2)} \), consistent with standard semi-classical arguments. (We stress that we will consider here only localized wave packets which are square-integrable, for which the evaluation of \( \Delta x_t \) and \( \Delta p_t \) is possible, and not pure plane wave states nor the special non-spreading, free-particle solutions discovered by Berry and Balazs \( \text{(13)} \).)

For the standard Gaussian or minimum uncertainty wave packet used in most textbook examples, and in fact for any initial wave packet of the form \( \psi(x, 0) = R(x) \exp(\text{i} p_0 (x - x_0)/\hbar) \) where \( R(x) \) is a real function, this initial correlation vanishes and the more familiar special case of \( \Delta x_t \) in Eqn. \( \text{(1)} \) results, leading many students to believe that it is the most general result possible. It is, however, very straightforward to construct initial quantum states consisting of simple Gaussian wave functions, such as squeezed states or linear combination of Gaussians, which have the required initial position-momentum correlations ‘built in’, and which therefore exhibit the general form in Eqn. \( \text{(2)} \), including examples where the position-space wave packet can initially shrink in width. Since these examples can be analyzed with little or no more mathematical difficulty than the standard minimum-uncertainty cases commonly considered in textbooks \( \text{(1)} \), we will focus on providing two such examples below. We will, however, also emphasize the utility of different ways of visualizing the time-dependent position-momentum correlations suggested by the form in Eqn. \( \text{(2)} \).

The derivation of Eqn. \( \text{(2)} \) has been most often discussed \( \text{(2), (8)} \) using the evaluation of the time-dependence of expectation values described by

\[
\frac{d}{dt} \langle \hat{A} \rangle = \frac{i}{\hbar} \langle [\hat{H}, \hat{A}] \rangle \tag{3}
\]

using the free particle Hamiltonian, \( \hat{H} = \hat{p}^2 / 2m \), or related matrix methods \( \text{(3)} \); since we are interested only in expectation values of operators (\( \hat{A} = \hat{x} \) or \( \hat{p} \)) which are themselves independent of time, there is no additional \( \langle d\hat{A}/dt \rangle \) term in Eqn. \( \text{(3)} \). In the next section, we derive the necessary time-dependent expectation values of powers of position and momentum in a complementary way, using very general momentum-space ideas. (Identical methods can then also be used to evaluate the general form of \( \Delta x_t \) for the related case of uniform acceleration, which we discuss in Appendix \( \text{[A]} \).) Then in Sec. \( \text{III} \) we briefly review the special case of the minimum-uncertainty Gaussian wave packet (to establish notation) focusing on the introduction of useful tools to help visualize possible correlations between position and momentum in free particle wave packets, especially the direct visualization of
the real/imaginary parts of $\psi(x, t)$, the time-dependent spatial distribution of kinetic energy, as well as the Wigner quasi-probability distribution. Then, in Sec. IV we exhibit two cases of correlated wave packets with the general form of $\Delta x_t$ in Eqn. (2), which are simple extensions of these standard results. A similar example, involving squeezed states, has been discussed in Ref. [14], but we will focus here on understanding the detailed position-momentum correlations which give rise to the term linear in $t$ in Eqn. (2), especially using the techniques outlined in Sec. III for their visualization. Finally, we make some concluding remarks as well as noting in an Appendix that very similar results (both for the general form of the time-dependent $\Delta x_t$ and for the exemplary cases studied here) can be obtained for the Schrödinger equation corresponding to the case of constant acceleration.

II. TIME-DEPENDENT $\Delta x_t$ USING MOMENTUM-SPACE WAVEFUNCTIONS

While the general result for the free-particle $\Delta x_t$ is most often obtained using formal methods involving the time-dependence of expectation values as in Eqn. (3), one can also evaluate time-dependent powers of position and momentum for a free particle in terms of the initial wave packet quite generally in terms of the momentum-space description of the quantum state, namely $\phi(p, t)$, obtaining the same results, in a manner which is nicely complementary to more standard analyses. Depending on the ordering of topics in a given quantum mechanics course syllabus, this discussion might well be applicable and understandable earlier in the curriculum than the more formal method.

In this approach, the most general momentum-space wave function which solves the free-particle time-dependent Schrödinger equation

$$\frac{p^2}{2m} \phi(p, t) = \hat{H} \phi(p, t) = \hat{E} \phi(p, t) = i\hbar \frac{\partial}{\partial t} \phi(p, t),$$

(4)

can be written in the form

$$\phi(p, t) = \phi_0(p) e^{-ip^2t/2m\hbar}$$

(5)

with $\phi(p, 0) = \phi_0(p)$ being the initial state wavefunction. The $t$-dependent expectation values for powers of momentum are trivial since

$$\langle \hat{p} \rangle_t = \int_{-\infty}^{+\infty} p \phi_0(p)^2 dp \equiv \langle \hat{p} \rangle_0$$

(6)

$$\langle \hat{p}^2 \rangle_t = \int_{-\infty}^{+\infty} p^2 \phi_0(p)^2 dp \equiv \langle \hat{p}^2 \rangle_0$$

(7)
\[(\Delta p_t)^2 = (\langle \hat{p}^2 \rangle_t - \langle \hat{p} \rangle^2_t) = (\langle \hat{p}^2 \rangle_0 - \langle \hat{p} \rangle^2_0) = (\Delta p_0)^2 \] 

(8)

as expected for a free-particle solution for which \(|\phi(p, t)|^2 = |\phi_0(p)|^2\) is independent of time.

In this representation, the position operator is given by the non-trivial form \(\hat{x} = i\hbar (\partial/\partial p)\), and the time-dependent expectation value of position can be written as

\[
\langle \hat{x} \rangle_t = \int_{-\infty}^{+\infty} [\phi(p, t)]^* \hat{x} [\phi(p, t)] dp \\
\quad = \int_{-\infty}^{+\infty} [\phi_0^*(p)] e^{+ip^2t/2m\hbar} \left( i\hbar \frac{\partial}{\partial p} \right) \left[ \phi_0(p) e^{-ip^2t/2m\hbar} \right] dp \\
\quad = \int_{-\infty}^{+\infty} [\phi_0^*(p)] \left( i\hbar \frac{\partial}{\partial p} \right) [\phi_0(p)] dp + \frac{t}{m} \int_{-\infty}^{+\infty} p |\phi_0(p)|^2 dp \\
\quad = \langle \hat{x} \rangle_0 + \frac{t}{m} \langle \hat{p} \rangle_0
\]

(9)

which is consistent with Ehrenfest’s theorem for the essentially classical behavior of \(\langle \hat{x} \rangle_t\).

The same formalism can be used to evaluate \(\langle \hat{x}^2 \rangle_t\) and gives

\[
\langle \hat{x}^2 \rangle_t = \langle \hat{x}^2 \rangle_0 + \frac{t}{m} \langle \hat{x} \hat{p} + \hat{p} \hat{x} \rangle_0 + \frac{t^2}{m^2} \langle \hat{p}^2 \rangle_0
\]

(10)

where one can use the general representation-independent commutation relation \([\hat{x}, \hat{p}] = i\hbar\) to simplify the answer to this form. The symmetric combination of position and momentum operators, written here as \((\hat{x} \hat{p} + \hat{p} \hat{x})\), which is obviously Hermitian, guarantees that this expression is manifestly real. (Discussions in textbooks on symmetrizing products of non-commuting operators abound, but such results are seldom put into the context of being useful or natural in specific calculations, as is apparent in their use here.)

Combining Eqns. (9) and (10) then gives the most general form for the time-dependent spread in position to be

\[
(\Delta x_t)^2 = (\langle \hat{x}^2 \rangle_t - \langle \hat{x} \rangle_t^2) = \left( \langle \hat{x}^2 \rangle_0 + \frac{t}{m} \langle \hat{x} \hat{p} + \hat{p} \hat{x} \rangle_0 + \frac{t^2}{m^2} \langle \hat{p}^2 \rangle_0 \right) - \left( \langle \hat{x} \rangle_0 + \frac{t}{m} \langle \hat{p} \rangle_0 \right)^2 \\
\quad = (\Delta x_0)^2 + \frac{t (\langle \hat{x} \hat{p} + \hat{p} \hat{x} \rangle_0 - 2\langle \hat{x} \rangle_0 \langle \hat{p} \rangle_0)}{m} + \frac{t^2}{m^2} \langle \hat{p}^2 \rangle_0 \\
\quad = (\Delta x_0)^2 + \left( \langle \hat{x} - \langle \hat{x} \rangle_0 \rangle \langle \hat{p} - \langle \hat{p} \rangle_0 \rangle + \langle \hat{p} - \langle \hat{p} \rangle_0 \rangle \langle \hat{x} - \langle \hat{x} \rangle_0 \rangle \right)\frac{t}{m} + \frac{t^2}{m^2} \langle \hat{p}^2 \rangle_0.
\]

(11)

We have rewritten the term linear in \(t\) in a form which stresses that it is a correlation between \(x\) and \(p\), similar in form to related classical quantities such as the covariance in
probability and statistics. Recall that for two classical quantities, \( A \) and \( B \), described by a joint probability distribution, the covariance is defined as

\[
cov(A, B) = \langle (A - \langle A \rangle)(B - \langle B \rangle) \rangle = \langle AB \rangle - \langle A \rangle \langle B \rangle.
\]

As we will see in the next section, there is no initial correlation for the familiar minimum-uncertainty Gaussian wave packets. However, for simple variations on the standard example, as in Sec. IV, we will find non-vanishing correlations, which we can visualize with the methods in Sec. III.

We stress that the notion of a time-dependent correlation between \( x \) and \( p \) at arbitrary times \( (t > 0) \) can be easily generalized from these results, and we can define a generalized covariance for these two variables \([10]-[12]\) (or any two operators, \( \hat{A}, \hat{B} \)) as

\[
cov(\hat{x}, \hat{p}; t) \equiv \frac{1}{2} \langle (\hat{x} - \langle \hat{x} \rangle_t)(\hat{p} - \langle \hat{p} \rangle_t) + (\hat{p} - \langle \hat{p} \rangle_t)(\hat{x} - \langle \hat{x} \rangle_t) \rangle_t \tag{13}
\]

where the additional factor of \( 1/2 \) accounts for the necessarily symmetric combination which appears, compared to the classical definition. One can then speak of a time-dependent correlation coefficient defined by

\[
\rho(x, p; t) \equiv \frac{\text{cov}(x, p; t)}{\Delta x \cdot \Delta p_t} \tag{14}
\]

in analogy with related quantities from statistics. This correlation can be shown \([12]\) to satisfy the inequality

\[
[\rho(x, p; t)]^2 \leq 1 - \left( \frac{|\langle [\hat{x}, \hat{p}] \rangle|}{2 \Delta x \cdot \Delta p_t} \right)^2 = 1 - \left( \frac{\hbar}{2 \Delta x \cdot \Delta p_t} \right)^2 \tag{15}
\]

which vanishes for the standard minimum-uncertainty Gaussian at \( t = 0 \), but which is non-zero for later times, as we will see below.

### III. STANDARD MINIMUM-UNCERTAINTY GAUSSIAN WAVE PACKETS

The standard initial minimum-uncertainty Gaussian wave packet, which gives the familiar time-dependent spread in Eqn. II, can be written in generality as

\[
\phi_0(p) = \phi_G(p, 0) = \sqrt{\frac{\alpha}{\sqrt{\pi}}} e^{-\alpha^2(p-p_0)^2/2} e^{-ipx_0/\hbar} \tag{16}
\]
where \( x_0, p_0 \) are used to characterize the arbitrary initial central position and momentum values respectively. This form gives

\[
\langle \hat{p} \rangle_t = p_0, \quad \langle \hat{p}^2 \rangle_t = p_0^2 + \frac{1}{2\alpha^2}, \quad \text{and} \quad \Delta p_t = \Delta p_0 = \frac{1}{\alpha \sqrt{2}} \tag{17}
\]

which are, of course, consistent with the general results in Eqns. (6) and (7).

The explicit form of the position-space wave function is given by Fourier transform as

\[
\psi_G(x, t) = \frac{1}{\sqrt{2\pi \hbar \sqrt{\pi} \alpha \sqrt{1 + (it/t_0)^2}}} e^{ip_0(x-x_0)/\hbar} e^{-(p-p_0)^2/(2\hbar)} e^{-i\hat{x}^2 t / 2m\hbar}, \tag{18}
\]

which can be evaluated in closed form (using the change of variables \( q \equiv p - p_0 \) and standard integrals) to obtain

\[
\psi_G(x, t) = \frac{1}{\sqrt{\pi \alpha \hbar (1 + it/t_0)}} e^{ip_0(x-x_0)/\hbar} e^{-i\hat{x}^2 t / 2m\hbar} e^{-(x-x_0-p_0t/m)^2 / 2(\alpha^2)(1+it/t_0)} \tag{19}
\]

where \( t_0 \equiv m\hbar \alpha^2 \) is the spreading time. This then gives

\[
|\psi_G(x, t)|^2 = \frac{1}{\sqrt{\pi \beta_t}} e^{-|x-\bar{x}(t)|^2 / \beta_t^2} \tag{20}
\]

where

\[
\bar{x}(t) \equiv x_0 + p_0 t/m \quad \text{and} \quad \beta_t \equiv \beta \sqrt{1 + (t/t_0)^2} \quad \text{with} \quad \beta \equiv \alpha \hbar. \tag{21}
\]

This gives

\[
\langle \hat{x} \rangle_t = \bar{x}(t) \quad \text{and} \quad \langle \hat{x}^2 \rangle_t = [\bar{x}(t)]^2 + \frac{\beta^2}{2}, \tag{22}
\]

so that

\[
(\Delta x_t)^2 = \frac{\beta^2}{2} = \frac{\beta^2}{2} \left(1 + \left(\frac{t}{t_0}\right)^2\right) = (\Delta x_0)^2 + (\Delta p_0 t/m)^2 \tag{23}
\]

which is the familiar textbook result, and for \( t = 0 \) has the minimum uncertainty product \( \Delta x_0 \cdot \Delta p_0 = \hbar/2 \).

It is easy to confirm by direct calculation that there is no initial \((t = 0) x - p\) correlation \((\text{cov}(x, p; 0) = 0)\) for this wavefunction, consistent with the lack of a term linear in \( t \) in Eqn. (23). We emphasize that such correlations do indeed develop as the wavepacket evolves in time, which can be seen by examining the form of either the real or imaginary parts of \( \psi_G(x, t) \) as shown in Fig. 1 (where we specify the model parameters used in that plot in the accompanying figure caption). We note that for times \( t > 0 \), the ‘front end’ of the wave packet shown there is clearly more ‘wiggly’ than the ‘back end’ (simply count the nodes
The time-dependent correlation function or covariance defined in Eqn. (13) and correlation coefficient from Eqn. (14) are easily calculated for this specific case to be

\[
\text{cov}(x, p; t) = \frac{\hbar}{2} \left( \frac{t}{t_0} \right) \quad \text{and} \quad \rho(x, p; t) = \frac{t/t_0}{\sqrt{1 + (t/t_0)^2}}
\]

which clearly expresses the increasingly positive correlation of fast (slow) momentum components being preferentially in the leading (trailing) edge of the wave packet. We note that such correlations have been discussed in Refs. [11] and [12].

This observation can also be described quantitatively by examining the distribution of kinetic energy of such a free-particle Gaussian wavepacket [15]. In this approach, the standard expression for the kinetic energy is rewritten using integration-by-parts in the form

\[
\langle \hat{T} \rangle_t = \frac{1}{2m} \langle \hat{p}^2 \rangle_t = -\frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} dx \psi^*(x, t) \frac{\partial^2 \psi(x, t)}{\partial x^2} = \frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} dx \left| \frac{\partial \psi(x, t)}{\partial x} \right|^2
\]

which can be used to define a local kinetic energy density, \( T(x, t) \), via

\[
T(x, t) \equiv \frac{\hbar^2}{2m} \left| \frac{\partial \psi(x, t)}{\partial x} \right|^2 \quad \text{where} \quad \langle \hat{T} \rangle_t = \int_{-\infty}^{+\infty} T(x, t) \, dx \equiv T(t).
\]

As this notion is useful in systems other than for free particle states, we allow for the possibility that the total kinetic energy varies with time. Since this local density is clearly real and positive-definite, we can use it to visualize the distribution of kinetic energy (or ‘wiggliness’) in any time-dependent wavefunction. We can then define similar quantities for the kinetic energy in the ‘front’ and/or ‘back’ halves of the wave packet, using \( \langle x \rangle_t \) as the measuring point, via

\[
T^{(+)}(t) \equiv \int_{\langle x \rangle_t}^{+\infty} T(x, t) \, dx \quad \text{and} \quad T^{(-)}(t) \equiv \int_{-\infty}^{\langle x \rangle_t} T(x, t) \, dx.
\]

For the standard Gaussian wave packet in Eqn. (19), the local kinetic energy density is given by

\[
T_G(x, t) = \frac{1}{2m} \left( \frac{p_0^2}{2} + \frac{[x - \bar{x}(t)]^2}{\alpha^2 \hbar} \right) \left[ \frac{t/t_0}{1 + t^2/t_0^2} \right] + \frac{[x - \bar{x}(t)]^2}{(\alpha^2 \hbar)^2(1 + t^2/t_0^2)} \right| \psi_G(x, t) |^2.
\]

The expectation value of the kinetic energy is correctly given by

\[
T_G(t) = \int_{-\infty}^{+\infty} T_G(x, t) \, dx = \frac{1}{2m} \left( p_0^2 + \frac{1}{2\alpha^2} \right)
\]
and receives non-zero contributions from only the first and last terms in brackets in Eqn. (28), since the term linear in \([x - \mathbf{x}(t)]\) vanishes (when integrated over all space) for symmetry reasons. The individual values of \(T_{(G)}^{(\pm)}(t)\) can also be calculated and are given by

\[
T_{(G)}^{(\pm)}(t) = \frac{1}{2m} \left( \frac{1}{2} \right) \left( \frac{p_0^2}{1^2} \right) \left( \frac{t/t_0}{1 + t^2/t_0^2} \right) + \frac{1}{2} \alpha^2
\]

which are individually positive definite. The time-dependent fractions of the total kinetic energy contained in the (+)/(-) (right/left) halves of this standard wave packet are given by

\[
R_{(G)}^{(\pm)}(t) \equiv \frac{T_{(G)}^{(\pm)}(t)}{T_{(G)}^{(+)}(t) + T_{(G)}^{(-)}(t)} = \frac{1}{2} \pm \left( \frac{2}{\sqrt{\pi}} \right) \left( \frac{(p_0 \alpha)}{(2(p_0 \alpha)^2 + 1)} \right) \frac{t/t_0}{1 + t^2/t_0^2}
\]

For the model parameters used in Fig. 1, for \(t = 2t_0\) this corresponds to \(R^{(+)} / R^{(-)} = 56\%/44\%\), consistent with the small, but obvious, difference in the kinetic energy distribution seen by ‘node counting’.

Finally, this growing correlation can be exhibited in yet another way, namely through the Wigner quasi-probability distribution, defined by

\[
P_W(x, p; t) \equiv \frac{1}{\pi \hbar} \int_{-\infty}^{+\infty} \psi^*(x + y, t) \psi(x - y, t) e^{+2ipy/\hbar} dy = \frac{1}{\pi \hbar} \int_{-\infty}^{+\infty} \phi^*(p + q, t) \phi(p - q, t) e^{-2ixq/\hbar} dq.
\]

This distribution, first discussed by Wigner [16], and reviewed extensively in the research [17] and pedagogical [18] literature (and even in the context of wave packet spreading [19]), is as close as one can come to a quantum phase-space distribution, and while not directly measurable, can still be profitably used to illustrate any \(x - p\) correlations. For the standard minimum-uncertainty Gaussian wavefunctions defined by Eqns. (16) or (19), one finds that

\[
P_W(x, p; t) = \frac{1}{\hbar \pi} e^{-(p-p_0)^2/\alpha^2} e^{-(x-x_0-pt/m)^2/\beta^2} = P_W(x - pt/m, p; 0).
\]

Contour plots of \(P_W(x, p; t)\) corresponding to the time-dependent standard Gaussian wave packet for two different times (\(t = 0\) and \(t = 2t_0\)) are also shown at the bottom of Fig. 1, where the the elliptical contours with principal axes parallel to the \(x, p\) axes for the \(t = 0\) case are indicative of the vanishing initial correlation, while the slanted contours at later times are consistent with the correlations developing as described by Eqn. (24). (We note that Bohm [11] uses a similar illustration, but discusses it only in the context of classical phase
space theory and Liouville’s theorem.) The visualization tools used in Fig. 1 (explicit plots of \( Re[\psi(x, t)] \), and the Wigner function) and the distribution of kinetic energy as encoded in Eqns. (30) or (31), can then directly be used to examine the correlated wave packets we discuss in the next section.

As a final reminder about the quantum mechanical “engineering” of model one-dimensional wavepackets, we recall that since an initial \( \phi_0(p) \) is related to the time-dependent \( \psi(x, t) \) for free-particle solutions via

\[
\psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \left[ \phi_0(p) e^{-ip^2t/2m\hbar} \right] e^{ipx/\hbar} dp \tag{35}
\]

then the simple modification

\[
\tilde{\phi}_0(p) = \phi_0(p) e^{-ipa/\hbar} e^{ip^2\tau/2m\hbar} \tag{36}
\]

leads to the related position-space wavefunction satisfying

\[
\tilde{\psi}(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \left[ \left( \phi_0(p) e^{-ip\alpha/\hbar} e^{ip^2\tau/2m\hbar} \right) e^{-ip^2t/2m\hbar} \right] e^{ipx/\hbar} dp = \psi(x - a, t - \tau) \tag{37}
\]

so that simple shifts in coordinate and time labels are possible, and squeezed states often make use of similar connections.

IV. CORRELATED GAUSSIAN WAVE PACKETS

A. Squeezed states

One of the simplest modifications of a standard minimum-uncertainty Gaussian initial state which induces non-trivial initial correlations between position and momentum is given by

\[
\phi_S(p, 0) = \sqrt{\frac{\alpha}{\sqrt{\pi}}} e^{-\alpha^2(p-p_0)^2(1+iC)/2} e^{-ipx_0/\hbar}. \tag{38}
\]

(A similar version of a squeezed state, but with \( \psi(x, 0) \) modified, has been discussed in Ref. [14].) Because the additional \( C \) term is a simple phase, the modulus of \( \phi(p, t) \) is unchanged so that the expectation values of momentum, \( \langle \hat{p} \rangle_0 \) and \( \langle \hat{p}^2 \rangle_0 \), and the momentum-spread, are still given by Eqn. [17] as for the standard Gaussian example. However, there is now an obvious coupling between the usual ‘smooth’ \( \exp(-\alpha^2(p-p_0)^2/2) \) term which describes the peak momentum values and the ‘oscillatory’ \( \exp(-ipx_0/\hbar) \) terms which dictates
the spatial location and spread, governed by the presence of the new $C$ term, which leads to a non-zero initial $x - p$ correlation.

The time-dependent position-space wavefunction is obtained via Fourier transform with literally no more work than for the standard Gaussian and one finds

$$
\psi_S(x,t) = \frac{1}{\sqrt{\pi \beta(1 + it)|C + (t/t_0)|}} e^{ip_0(x-x_0)/\hbar} e^{-ip_0^2 t/2\hbar m} e^{-(x-x_0-p_0 t/m)^2/(2\beta^2(1+i|C+t/t_0|))} \quad (39)
$$

giving

$$
|\psi_S(x,t)|^2 = \frac{1}{\sqrt{\pi b(t)}} e^{-\left[x - \bar{x}(t)\right]^2/b^2(t)} \quad \text{where} \quad b(t) \equiv \beta \sqrt{1 + (C + t/t_0)^2}. \quad (40)
$$

Thus, the initial state in Eqn. (38) gives the same time-dependent Gaussian behavior as the standard case, still peaked at $x = \bar{x}(t)$, but with a spatial width shifted in time from $t \rightarrow t + Ct_0$. This can be understood from the results in Eqns. (36) and (37) where the new $C$-dependent terms in Eqn. (38) give rise to effective $a$ and $\tau$ shifts given by

$$
a = -C\alpha^2 \hbar p_0 \quad \text{and} \quad \tau = -C\alpha^2 m \hbar = -Ct_0. \quad (41)
$$

The $\tau$ shift then affects the time-dependent width, $b(t)$, but the combined $a, \tau$ shifts undo each other in the argument of the Gaussian exponential because they are highly correlated due to the form in Eqn. (38).

The time-dependent position expectation values are then

$$
\langle \hat{x} \rangle_t = \bar{x}(t) \quad \text{and} \quad \langle \hat{x}^2 \rangle_t = [\bar{x}(t)]^2 + \frac{[b(t)]^2}{2}, \quad (42)
$$

so that

$$
(\Delta x_t)^2 = \frac{[b(t)]^2}{2} = \frac{\beta^2}{2} \left(1 + (C + t/t_0)^2 \right) = \frac{\beta^2}{2} \left(1 + C^2 \right) + \frac{C\beta^2 t_0}{t_0} + \frac{\beta^2 t_0^2}{2t_0^2} = (\Delta x_0)^2 + At + \frac{(\Delta p_0)^2 t_0^2}{m^2} \quad (43)
$$

which has a non-vanishing linear term if $C \neq 0$. The initial width of this packet is larger than for the minimal uncertainty solution by a factor of $\sqrt{1 + C^2}$, but has the same quadratic time-dependence since $\Delta p_0$ is the same.

One can confirm by direct calculation that $\phi_S(p,0)$ and $\psi_S(x,0)$ both do have an initial non-vanishing correlation leading to this form and this is also clear from plots of the initial
wave packet as shown in Fig. 2. We plot there an example with the same model parameters as in Fig. 1, but with \( C = -2 \) which leads to an anti-correlation (since \( C < 0 \)) with higher momentum components (more wiggles) in the ‘back edge’ of the initial packet. This gives an intuitive expectation for a wave packet which initially shrinks in time, consistent with the result in Eqn. (43), and with the plot shown in Fig. 2 for \( t = 2t_0 \). The parameters were chosen such that for this time the initial correlation has become ‘undone’, leading to something like the standard Gaussian initial state, from which point it spreads in a manner which is more familiar. The initial correlation is achieved, however, at the cost of increasing the initial uncertainty principle product by a factor of \( \sqrt{1 + C^2} \). The complete time-dependent correlation coefficient from Eqn. (14) is

\[
\rho(x, p; t) = \frac{(C + t/t_0)}{\sqrt{1 + (C + t/t_0)^2}}
\]

(44)
corresponding in this case to a roughly 90% initial correlation. The required initial correlation is also clearly evident from the Wigner quasi-probability distribution for this case, where we find

\[
P_W(x, p; t) = \frac{1}{\hbar \pi} e^{-\beta (p - p_0)^2 \alpha^2} e^{-\left(x - x_0 - pt/m - C(p - p_0)t_0/m\right)^2/\beta^2}.
\]

(45)
In this case, the initial correlation for \( C < 0 \) shown in Fig. 2 is consistent with the desired anti-correlation, since the slope of the elliptical contours is negative.

In a very similar manner, the expressions for the kinetic energy density distribution from Eqn. (31) are simply shifted to

\[
R^{(\pm)}(S)(t) \equiv \frac{T^{(\pm)}(S)(t)}{T^{(+)}(S)(t) + T^{(-)}(S)(t)} = \frac{1}{2} \pm \left( \frac{2}{\sqrt{\pi}} \right) \left( \frac{\alpha}{(2\alpha^2 + 1)} \right) \frac{(C + t/t_0)}{\sqrt{1 + (C + t/t_0)^2}}
\]

(46)
so that for \( C < 0 \), there is an initial asymmetry in the front/back kinetic energy distribution, with more ‘wiggles’ in the trailing half of the packet. For the \( C = -2 \) case in Fig. 2, the initial \((t = 0)\) front/back asymmetry is \( R^{(+)} / R^{(-)} = 44\% / 56\% \).

We note that while a number of quantities (time-dependent spread in position, correlation coefficient, kinetic energy distribution) are simply obtained by the \( t \to t + Ct_0 \) shift, other important metrics, such as the autocorrelation function \([21], A(t)\), retain basically the same form.

One can imagine generating initial Gaussian states with non-zero correlations of the type in Eqn. (38), motivated by results obtained by the use of modern atom trapping techniques,
such as in Ref. [22]. In a number of such experiments, harmonically bound ions are cooled to essentially their ground state, after which changes in the external binding potential can generate various nonclassical motional states such as coherent states (by sudden shifts in the central location of the binding potential [23]) and squeezed states (by changing the strength of the harmonic binding force, i.e., the spring constant). The subsequent time-development of Gaussian packets in such states can then lead to the desired correlated states, at which point the external binding potential can be suddenly removed, with free-particle propagation thereafter.

As an example, the initial state in a harmonic oscillator potential of the form $V(x) = \frac{m\omega^2 x^2}{2}$ given by

$$\psi(x, 0) = \frac{1}{\sqrt{\beta \sqrt{\pi}}} e^{ip_0 x/\hbar} e^{-x^2/2\beta^2}$$

(47)
evolves in time as

$$\psi(x, t) = \exp \left[ \frac{im\omega x^2 \cos(\omega t)}{2\hbar \sin(\omega t)} \right] \frac{1}{\sqrt{A(t) \sqrt{\pi}}} \exp \left[ - \frac{im\omega \beta x^2}{2\hbar \sin(\omega t)} \frac{(x - x_s(t))^2}{A(t)} \right]$$

(48)

where

$$A(t) \equiv \beta \cos(\omega t) + i \left( \frac{\hbar}{m\omega \beta} \right) \sin(\omega t) \quad \text{and} \quad x_s(t) \equiv \frac{p_0 \sin(\omega t)}{m\omega}.$$ 

(49)

The time-dependent expectation values are then

$$\langle x \rangle_t = x_s(t), \quad \Delta x_t = \frac{|A(t)|}{\sqrt{2}}, \quad \text{and} \quad \langle p \rangle_t = p_0 \cos(\omega t)$$

(50)

and it is then easy to show that the time-dependent correlation of this state is given by

$$\text{cov}(x, p; t) = \frac{m\omega \sin(\omega t) \cos(\omega t)}{2} \left[ \left( \frac{\hbar}{m\omega \beta} \right)^2 - \beta^2 \right].$$

(51)

For the special case of coherent states, where $\beta = \sqrt{\hbar/m\omega}$, the correlations vanish identically for all times (as does the asymmetry in kinetic energy [15]), while for more general solutions, removing the potential at times other than integral multiples of $\tau/2$ (where $\tau$ is the classical period) would yield an initially correlated Gaussian.

**B. Linear combinations of Gaussian solutions**

One of the simplest examples of correlated position-momentum behavior of a system, leading to an initial shrinking of a spatial width, can be classically modelled by two 1D
non-interacting particles, with the faster particle placed initially behind the slower one. A quantum mechanical solution of the free-particle Schrödinger equation involving simple Gaussian forms which mimics this quasi-classical behavior, and for which all expectation values and correlations can be evaluated in simple closed form, consists of a linear combination of two minimal-uncertainty Gaussian solutions of the form

\[
\psi_2(x, t) = N \left[ \cos(\theta) \psi_{(G)}^{(A)}(x, t) + \sin(\theta) \psi_{(G)}^{(B)}(x, t) \right] \tag{52}
\]

where \(A, B\) correspond to two different sets of initial position and momentum parameters, namely \((x_A, p_A)\) and \((x_B, p_B)\), \(\theta\) describes the relative weight of each component, and \(N\) is an overall normalization; we assume for simplicity that each component Gaussian has the same initial width, \(\beta\). Since each \(\psi_{(G)}(x, t)\) is separately normalized, the value of \(N\) can be easily evaluated using standard Gaussian integrals with the result that

\[
N^{-2} = 1 + \sin(2\theta) e^{-\frac{(x_A-x_B)^2}{4\beta^2}-\frac{(p_A-p_B)^2}{4\hbar^2}} \cos\left[(x_B - x_A)(p_B + p_A)/2\hbar\right] \tag{53}
\]

so that if the two initial Gaussians are far apart in phase space, namely if

\[
\frac{(x_A - x_B)^2}{4\beta^2} + \frac{(p_A - p_B)^2}{4\hbar^2} \gg 1, \tag{54}
\]

the normalization factor \(N\) can be effectively set to unity, and all cross-terms in the evaluation of expectation values can also be neglected.

In this limit, the various initial expectation values required for the evaluation of the time-dependent spread in Eqn. (2) are given by

\[
\langle \hat{x} \rangle_0 = \cos^2(\theta)x_A + \sin^2(\theta)x_B \tag{55}
\]

\[
\langle \hat{x}^2 \rangle_0 = \cos^2(\theta) \left( x_A^2 + \frac{\beta^2}{2} \right) + \sin^2(\theta) \left( x_B^2 + \frac{\beta^2}{2} \right) - \left[ \cos^2(\theta)x_A + \sin^2(\theta)x_B \right]^2 \tag{56}
\]

so that

\[
(\Delta x_0)^2 = [\sin(2\theta)]^2 \left( \frac{x_A - x_B}{2} \right)^2 + \frac{\beta^2}{2} \tag{57}
\]

with a similar result for the momentum-spread, namely

\[
(\Delta p_0)^2 = [\sin(2\theta)]^2 \left( \frac{p_A - p_B}{2} \right)^2 + \frac{\hbar^2}{2\beta^2}. \tag{58}
\]

The necessary initial correlation is given by

\[
\langle \hat{x} \hat{p} + \hat{p} \hat{x} \rangle_0 - 2\langle \hat{x} \rangle_0 \langle \hat{p} \rangle_0 = 2[\sin(2\theta)]^2 \left[ \frac{(x_A - x_B)(p_A - p_B)}{4} \right] \tag{59}
\]
so that the time-dependent spread in position is given by

\[ (\Delta x_t)^2 = [\sin(2\theta)]^2 \left( \frac{x_A - x_B}{2} + \left( \frac{p_A - p_B}{2} \right) \frac{t}{m} \right)^2 + \frac{\beta^2}{2} + \frac{\hbar^2 t^2}{2m^2\beta^2}. \]  

(60)

In the limit we’re considering, namely when \( |x_A - x_B| >> \beta \) and/or \( |p_A - p_B| >> \hbar/\beta \), the time-dependent width can be dominated by the quasi-classical value dictated by two well-separated ‘lumps’ of probability, and if \((x_A - x_B)\) and \((p_A - p_B)\) have opposite signs, then this large position spread can initially decrease in time because of the initial correlations. This example, while not as ‘quantum mechanical’ as that in Sec. IV A, does clearly and simply exhibit the position-momentum correlations necessary for the presence of the \( A \) term in Eqn. (43), with the ‘fast one in the back, and the slow one in the front’.

One can imagine producing linear combinations of isolated, but highly correlated, Gaussian wave packets at very different points in phase space, by invoking the dynamical time-evolution of bound state wave packets which leads to the phenomenon of wave packet revivals, especially fractional revivals [25]. For the idealized case of the infinite square well potential [26], at \( t = T_{rev}/4 \) (where \( T_{rev} \) is the full revival time), an initially localized wave packet is ‘split’ into two smaller copies of the original packet, located at opposite ends of phase space [27], of the form in Eqn. [52]. If, in this model system, the infinite wall boundaries are suddenly removed at such a point in time, we then have the case considered in this section.

V. CONCLUSION AND DISCUSSION

The study of the time-dependence of the spatial width of wave packets in model systems can produce many interesting results, a number of which are quasi-classical in origin, while some are explicitly quantum mechanical. Time-dependent wave packet solutions of the Schrödinger equation for the harmonic oscillator are easily shown to exhibit intricate correlated expansion/contraction of widths in position- and momentum-space [24] and modern experiments [22], [23] can probe a wide variety of such states. Even the behavior of otherwise free Gaussian wavepackets interacting with (or ‘bouncing from’) an infinite wall [28], [29], [30] can lead to wave packets which temporarily shrink in size.

While the fact that free-particle wavepackets can also exhibit initial shrinking of their spatial width is well-known in the physics pedagogical literature, it is perhaps not appre-
associated enough in the context of introductory quantum mechanics courses because of the seeming lack of simple, mathematically tractable, and intuitively visualizable examples, and we have provided two such simple cases here. We have also emphasized the usefulness of several tools for the detailed analysis of the structure of quantum states as they evolve, namely the direct visualization of the real/imaginary part of the spatial wavefunction, the time-dependent spatial distribution of the kinetic energy (how the ‘wiggliness’ changes in time), and the Wigner quasi-probability distribution all of which provide insight into the correlated $x - p$ structure of quantum states.

**APPENDIX A: TIME-DEPENDENT $\Delta x_t$ FOR THE CASE OF UNIFORM ACCELERATION**

Many of the results discussed here for the time-dependent widths of localized quantum wavepackets for the free-particle case can be carried over to the situation of a particle undergoing uniform acceleration, governed by the Hamiltonian $\hat{H} = \hat{p}^2/2m - Fx$, corresponding to a constant force, $+F$, to the right. General expressions for the time-dependent values of expectation values of powers of both $x$ and $p$ can be obtained using Eqn. (3) (following the method of Styer [8] for example) and one obtains the results

$$\langle \hat{p} \rangle_t = Ft + \langle p \rangle_0 \quad \text{and} \quad \langle \hat{p}^2 \rangle_t = F^2t^2 + 2F\langle \hat{p} \rangle_0 t + \langle \hat{p}^2 \rangle_0$$

which imply that $(\Delta p_t)^2 = (\Delta p_0)^2$. For position we have the corresponding results

$$\langle \hat{x} \rangle_t = \frac{Ft^2}{2m} + \frac{\langle \hat{p} \rangle_0 t}{m} + \langle \hat{x} \rangle_0$$

$$\langle \hat{x}^2 \rangle_t = \frac{F^2t^4}{4m^2} + \frac{F\langle \hat{p} \rangle_0 t^3}{m^2} + \frac{\langle \hat{p}^2 \rangle_0 t^2}{m^2} + \frac{F\langle \hat{x} \rangle_0 t^2}{m} + \frac{\langle \hat{x} \hat{p} + \hat{p} \hat{x} \rangle_0 t}{m} + \langle \hat{x}^2 \rangle_0$$

which actually combine to give the same expression for $(\Delta x_t)^2$ as in Eqn. (2). Thus, the model systems we have discussed here can also be used as examples of correlated wave packets in the related accelerating particle case.

The expressions above can also be derived using an approach similar to that followed in Sec. III namely by using the most general form for the time-dependent momentum-space wavefunction, $\phi(p, t)$. In that case, the time-dependent Schrödinger equation in $p$-space is written in the form

$$\frac{p^2}{2m} \phi(p, t) + F \left[ i\hbar \frac{\partial}{\partial p} \right] \phi(p, t) = i\hbar \frac{\partial}{\partial t} \phi(p, t)$$

(A4)
which has a general solution

\[ \phi(p, t) = \phi_0(p - Ft) e^{i[(p - Ft)^3 - p^3]/6mF} \]

(A5)

where \( \phi_0(p) = \phi(p, 0) \) is still the initial wavefunction. The \( t \)-dependent expectation values in Eqs. (6), (7), (9), and (10) can then be obtained as in Sec. II in terms of the \( t = 0 \) results, just as for Eqns. (6), (7), (9), and (10).
Figure Captions

Fig. 1. The time-development of a standard Gaussian wavepacket, $\psi_{(G)}(x,t)$, described by Eqn. (19), with the modulus (solid) and real part (dashed) shown for $t = 0$ and $t = 2t_0$ on the top plot. Contour plots of the Wigner function, from Eqn. (34), for the same two times are shown at the bottom, corresponding to contours which are 70%, 30%, and 10% of the peak or central value. The model parameters used in this plot are $\hbar = m = 1$ and $\beta = 2$, which give $t_0 \equiv m\beta^2/\hbar = 4$, along with $p_0 = 4$ and $x_0 = -4$ for the initial packet.

Fig. 2. Same as Fig. 1, but for the correlated squeezed state in Eqn. (38) or (39), with the model parameters used in Fig. 1. For this case, we use $C = -2$, so that for $t = 2t_0$ the initial correlations are ‘undone’.
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\(|\psi(x,t)|\) (solid) and Re[\(\psi(x,t)\)] (dashed) vs. \(x\)

contour plot of \(P_w(x,p;t)\) vs. \((x,p)\)

FIG. 1:
\[ |\psi(x, t)| \text{ (solid) and } \text{Re}[\psi(x, t)] \text{ (dashed) vs. } x \]

FIG. 2: Contour plot of \( P_w(x, p; t) \) vs. \((x, p)\)