*Electronic Research Archive*

http://www.aimspress.com/journal/era

ERA, 31(9): 5541–5558.
DOI: 10.3934/era.2023281
Received: 15 June 2023
Revised: 16 July 2023
Accepted: 02 August 2023
Published: 14 August 2023

*Research article*

# Eigenvalues and eigenvectors for a hermitian gaussian operator: Role of the Schrödinger-Robertson uncertainty relation

**R. F. Snider***

Department of Chemitry, University of British Columbia, Vancouver, BC, V6T 1Z1, Canada

* **Correspondence:** Email: rfsnider@shaw.ca.

**Abstract:** The eigenvalues and eigenvectors of a normalized gaussian operator do not seem to have been previously considered. I solve this problem for 1-dimensional translational systems. I also address the question as to whether a gaussian operator is a density operator. To answer that question, it is first necessary to be sure what conditions must be satisfied, so a short review of density operators is given. Since position and momentum do not commute in quantum mechanics, it is useful to start with the consequences of the noncommutation, which is generally the Schrödinger-Robertson uncertainty relation, which is also briefly reviewed. It is found that the question of whether a gaussian operator is a density operator is directly tied to this uncertainty relation. Since the Wigner function is the phase space representation of a translational density operator, it is natural to consider the gaussian phase space function associated with a gaussian operator and to compare the phase space and operator properties. Throughout such discussions, the independent parameters in these functions are the first and second moments of position and momentum. The application of this formalism to the free translation and spreading of a gaussian packet is given and shows the formal similarity between classical and quantum behavior, whereas the literature standardly only considers the pure state case (equivalent to a single wavefunction).

**Keywords:** eigenvalue; eigenvector; gaussian; density operator

## 1. Introduction

Gaussians play an important role in various aspects of physics as well as in the development of physical principles. In quantum mechanics, gaussian wavefunctions are used in a variety of ways, ranging from being a useful computational tool [1, 2] to being the structure of coherent states [3]. However, seemingly no or negligible use of gaussians in the structure of density operators appears in the literature. Here, this is explored to the extent of asking when a hermitian gaussian function $\langle x|G|y\rangle$ in two positions $x, y$ (which can be interpretated as the matrix representation of some quantum operator

$G$) is the representation of a density operator. What criterion is involved? Clearly it should have unit trace but is that enough? It is shown that the condition is whether expectations calculated when treating the matrix as a density matrix satisfies the Schrödinger-Robertson uncertainty principle [4–7]. Since the required expectation values for the uncertainty are moments of the position and momentum operators, it is useful to consider the phase-space representation of $G$, obtained by the inverse of the Weyl quantization [8,9], which defines the Wigner function [10] if $G$ is a density operator. The relations and properties of these different representations of $G$ are discussed in this paper.

The basic properties of density operators [11] is reviewed in the following subsection while the basic properties of the Schrödinger-Robertson uncertainty relation is reviewed in the subsequent subsection. These cover the technical aspects of these topics that are used in this paper. Section 2 discusses the relations between the different representations for the gaussian function and those position and momentum moments that parameterize the gaussian. It also classifies whether the gaussian has a quantum interpretation and if so, whether it is a pure or mixed density operator. Section 3 finds the eigenvalues and eigenvectors for the gaussian. This does not seem to have previously been done in the literature and some comment on related work is made. Section 4 explores the free particle time evolution of the gaussian and explores how, as a packet, it behaves as it passes past a fixed position. This has recently been considered by detailed computation [12, 13], which showed that, for certain parameterizations, the passage of the packet decreases with time during initial times. Here, the equation for the evolving packet is explicitly written down and it shows that a reversal of evolution can occur near the end of the packet's motion as well as at initial times. Only the latter was considered in [12, 13], and then only for a wave function.

### *1.1. Review of density operators*

Von Neumann [14] recognized that the proper mathematical formulation of wave functions was as elements of hilbert space and also introduced density operators as linear functionals (mappings) of quantum mechanical observables to their expectation values. Fano's paper [11] gives an elementary presentation of these ideas. Since quantum observables are hermitian (more correctly self-adjoint) operators, and thus have real eigenvalues, a density operator $\rho$ must be a positive hermitian operator with unit trace, so that an expectation value $\langle A\rangle_\rho = \mathrm{Tr}A\rho$ of $A$ is real [Tr stands for trace and the calculation is the same as if $A$ and $\rho$ were matrices]. In detail, if $A$ has eigenvalues $a_j$ and corresponding eigenvectors $|a_j\rangle$ with position representation $\psi_{a_j}(x) \equiv \langle x|a_j\rangle$, that is

$$A|a_j\rangle = a_j|a_j\rangle, \tag{1.1}$$

then $A$ has the spectral representation

$$A = \sum_j |a_j\rangle a_j\langle a_j|, \tag{1.2}$$

or in position representation

$$\langle x|A|y\rangle = \sum_j \langle x|a_j\rangle a_j\langle a_j|y\rangle = \sum_j \psi_j(x)a_j\psi^*(y), \tag{1.3}$$

on the basis that the eigenvectors are orthonormal, namely

$$\langle a_j|a_k\rangle = \int \psi_j^*(x)\psi_k(x)dx = \delta_{jk}. \tag{1.4}$$

Then the expectation of $A$ in state (density operator) $\rho$ is

$$\begin{aligned} \mathrm{TrA}\rho &= \langle A\rangle_\rho = \mathrm{Tr}\sum_{\mathrm{j}} |\mathrm{a_j}\rangle \mathrm{a_j}\langle \mathrm{a_j}|\rho \\ &= \sum_j a_j\langle a_j|\rho|a_j\rangle = \sum_j a_j p_{a_j} \end{aligned} \tag{1.5}$$

where the last form introduces the probability $p_{a_j} = \langle a_j|\rho|a_j\rangle$ of the system (that which is described by $\rho$) is in the $j$th eigenstate of $A$. To be a probability $p_{a_j}$ must be positive and less than 1. Since this has to be valid for any observable $A$, it is equivalent to the requirement that

$$1 \geq \langle\phi|\rho|\phi\rangle = \iint \phi^*(x)\langle x|\rho|y\rangle\phi(y)dxdy \geq 0, \tag{1.6}$$

for any normalized ($\langle\phi|\phi\rangle = 1$) square integrable wavefunction (element of hilbert space). An alternate way of viewing this is that, if $A = P_j \equiv |a_j\rangle\langle a_j|$ is the projection observable $P_j$ that asks what part of the state $\rho$ of the system is in state $|a_j\rangle$, then the expectation of this observable is

$$\langle P_j\rangle_\rho = \mathrm{Tr}|\mathrm{a_j}\rangle\langle \mathrm{a_j}|\rho = \langle \mathrm{a_j}|\rho|\mathrm{a_j}\rangle, \tag{1.7}$$

namely is the probability of being in $|a_j\rangle$ and as a probability must be $\geq 0$.

As a hermitian operator $\rho$ has eigenvalues $\rho_j$ and eigenvectors $|\chi_j\rangle$. namely

$$\rho|\chi_j\rangle = \rho_j|\chi_j\rangle. \tag{1.8}$$

The eigenvectors must be orthogonal for different eigenvalues

$$\langle\chi_j|\chi_k\rangle = 0 \quad \text{for} \quad \rho_j \neq \rho_k, \tag{1.9}$$

but generally eigenvalues may be degenerate, that is, two or more eigenvectors may have the same eigenvalue and can, for convenience, be chosen to be orthogonal, but this is not discussed further here. More important is that the expectation of the identity $\langle\mathbf{1}\rangle_\rho$ must be 1 so that the trace of $\rho$ is 1. Mathematically, this implies that $\rho$ must be of "trace class" and the spectrum of $\rho$ must be discrete (no continuous range of eigenvalues) [15]. Thus, its spectral representation is

$$\rho = \sum_j |\chi_j\rangle\rho_j\langle\chi_j|, \tag{1.10}$$

or in position representation (density matrix)

$$\langle x|\rho|y\rangle = \sum_j \chi_j(x)\rho_j\chi_j^*(y) \tag{1.11}$$

where $\chi_j(x) = \langle x|\chi_j\rangle$ is the position representation of $|\chi_j\rangle$. Equation (1.10) describes $\rho$ as being represented by a diagonal matrix whose trace is

$$\mathrm{Tr}\rho = \sum_{\mathrm{j}} \rho_{\mathrm{j}} = 1, \tag{1.12}$$

and interprets the eigenvalues $\rho_j$ of $\rho$ as the probabilities $\rho_j = p_j$ of the system being in the respective eigenstates $|\chi_j\rangle$, equivalently eigenfunctions $\chi_j(x)$, of $\rho$, again assuming the eigenvectors are normalized, $\langle\chi_j|\chi_j\rangle = 1$. Note the difference between the probabilities $p_j$ and $p_{a_j}$. Returning to the positivity condition of Eq (1.6), for any $\phi$, this condition is

$$\langle\phi|\rho|\phi\rangle = \sum_j \langle\phi|\chi_j\rangle\rho_j\langle\chi_j|\phi\rangle = \sum_j \rho_j|\langle\chi_j|\phi\rangle|^2 \geq 0, \tag{1.13}$$

requiring $\rho_j \geq 0$ for all eigenvalues $\rho_j$. Thus knowing the eigenvalues of $\rho$ is a method of verifying whether $\rho$ is a valid density operator.

### *1.2. Review of the Schrödinger-Robertson uncertainty relation*

The uncertainty relation is due to the commutation relation of momentum and position, namely $[p, x] \equiv (px - xp) = \hbar/i$. Here, $p$ and $x$ are quantum mechanical operators and no particular notation will be used to distinguish them from their classical analogs so it is only in the context of how they are used that distinguishes whether a quantum or classical meaning applies. The first and second moments of $p$ and $x$ are the expectation values

$$\begin{aligned} &\langle p\rangle,\ \ \langle x\rangle,\ \ \sigma^{(02)} \equiv \langle(p - \langle p\rangle)^2\rangle,\ \ \sigma^{(20)} \equiv \langle(x - \langle x\rangle)^2\rangle, \\ &\sigma^{(11)} \equiv \langle\frac{1}{2}[(p - \langle p\rangle)(x - \langle x\rangle) + (x - \langle x\rangle)(p - \langle p\rangle)]\rangle. \end{aligned} \tag{1.14}$$

These are also referred to as respectively, the mean momentum, mean position, momentum variance, position variance and the position-momentum covariance. It is the anticommutator of momentum and position that appears in the latter so that all moments are real valued. The standard deviations of momentum and position are $\sigma_p \equiv \sqrt{\sigma^{(02)}}$ and $\sigma_x \equiv \sqrt{\sigma^{(20)}}$ and are the quantities usually referred to in statistical arguments. Note that all second order moments involve differences of the variable from its corresponding mean value. All these quantities could be applied to 2- or 3-dimensional systems but for simplicity only the 1-dimensional case is discussed here.

The expectation value of the nonhermitian operator $(x - \langle x\rangle)(p - \langle p\rangle)$ can be arranged into antihermitian and hermitian contributions [4, 6, 7, 16]

$$\begin{aligned} \langle(x - \langle x\rangle)(p - \langle p\rangle)\rangle &= \frac{1}{2}\langle(x - \langle x\rangle)(p - \langle p\rangle) - (p - \langle p\rangle)(x - \langle x\rangle)\rangle \\ &\quad + \frac{1}{2}\langle(x - \langle x\rangle)(p - \langle p\rangle) + (p - \langle p\rangle)(x - \langle x\rangle)\rangle \\ &= i\hbar/2 + \sigma^{(11)}, \end{aligned} \tag{1.15}$$

with useful evaluations. Schwartz's inequality for states,

$$\langle\phi|\psi\rangle \leq \sqrt{\langle\phi|\phi\rangle\langle\psi|\psi\rangle} \tag{1.16}$$

can be generalized to mixed states with hermitian operators $A$ and $B$,

$$\langle AB\rangle_\rho \equiv \sum_j p_j\langle\chi_j|AB|\chi_j\rangle = \sum_j p_j\langle A\chi_j|B\chi_j\rangle$$
$$\leq \sum_j p_j\sqrt{\langle\chi_j|A^2|\chi_j\rangle\langle\chi_j|B^2|\chi_j\rangle} \leq \sqrt{\langle A^2\rangle_\rho\langle B^2\rangle_\rho}, \tag{1.17}$$

using the hermiticity of each of $A$ and $B$, and finally putting $p_j$ into the square root and allowing the independent sums over the index $j$ within the square root [16]. Combining the absolute square values of Eqs (1.15) and (1.17) while using $A = x - \langle x\rangle$ and $B = p - \langle p\rangle$ in the latter gives the Schrödinger-Robertson uncertainty relation [4, 6, 7, 16]

$$|\langle(x - \langle x\rangle)(p - \langle p\rangle)\rangle|^2 = \frac{\hbar^2}{4} + [\sigma^{(11)}]^2 \leq \sigma^{(20)}\sigma^{(02)}. \tag{1.18}$$

There are different ways of writing this inequality. What is found particularly useful when finding the eigenvalues and eigenvectors of a gaussian operator is

$$U \equiv \sqrt{\sigma^{(20)}\sigma^{(02)} - [\sigma^{(11)}]^2} \geq \frac{\hbar}{2}. \tag{1.19}$$

This is referred to as the "covariance-free uncertainty relation" in the following sections of this paper. Note that if there is no position-momentum covariance, this reduces to the standard Heisenberg uncertainty relation

$$U = \sigma_x\sigma_p \geq \frac{\hbar}{2} \tag{1.20}$$

involving the standard deviations rather than the variances. The latter is the uncertainty relation that is usually quoted for all cases by ignoring the possible role of the covariance.

## 2. When is a Gaussian operator a density operator

It is to be understood that a hermitian gaussian operator $G$ is an operator whose position representation $\langle x|G|y\rangle$ is a gaussian in $x$ and $y$. An obvious choice of writing this is as a linear combination of $x, y, x^2, y^2$ and $xy$ in the exponent but the calculation of the moments relative to the mean position and momentum is lengthy with this choice. A more convenient choice is to expand using the powers of the differences $x - \langle x\rangle$ and $y - \langle x\rangle$ in the exponent, thus

$$\langle x|G|y\rangle = N\exp\left[-g(x - \langle x\rangle)^2 - g^*(y - \langle x\rangle)^2 - g_1(x - \langle x\rangle)(y - \langle x\rangle) - ig_2(x - y)\right]. \tag{2.1}$$

Note, there is only one mean position $\langle x\rangle$ and the difference $x - y$ could be written with the mean position subtracted for each $x$ and $y$, but these cancel out. This involves 5 real parameters since $g = g_R + ig_I$ has independent real and imaginary parts, while $g_1$, $g_2$ and $\langle x\rangle$ are real and the manner in which the equation is written is to be consistent with hermiticity, namely $\langle x|G|y\rangle = \langle y|G|x\rangle^*$. The normalization constant $N$ is determined to make the trace of $G$, equivalent to the integral over the diagonal elements of $G$, equal to 1, namely

$$\int_{-\infty}^{\infty}\langle x|G|x\rangle dx = 1, \tag{2.2}$$

it being assumed that the range of positions is $[-\infty, \infty]$. The integral is easily evaluated since the integrand is just a Gaussian,

$$N\int_{-\infty}^{\infty}\exp[-(2g_R+g_1)(x-\langle x\rangle)^2]dx = N\sqrt{\frac{\pi}{2g_R+g_1}} = 1, \tag{2.3}$$

implying

$$N = \sqrt{\frac{2g_R+g_1}{\pi}}. \tag{2.4}$$

The moments are given by

$$\begin{aligned}
\langle x\rangle &= \int_{-\infty}^{\infty} x\langle x|G|x\rangle dx = \langle x\rangle, \quad \sigma^{(20)} = \int_{-\infty}^{\infty}(x-\langle x\rangle)^2\langle x|G|x\rangle dx = \frac{1}{2(2g_R+g_1)},\\
\langle p\rangle &= \int_{-\infty}^{\infty}\frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|G|y\rangle\Big|_{y=x}dx = \frac{\hbar}{i}\int_{-\infty}^{\infty}[-2g(x-\langle x\rangle)-g_1(y-\langle x\rangle)-ig_2]\langle x|G|y\rangle\Big|_{y=x}dx = -\hbar g_2,\\
\sigma^{(02)} &= \langle p^2\rangle - \langle p\rangle^2 = -\hbar^2\int_{-\infty}^{\infty}\frac{\partial^2}{\partial x^2}\langle x|G|y\rangle\Big|_{y=x}dx - \hbar^2 g_2^2\\
&= -\hbar^2\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\Big[\{-2g(x-\langle x\rangle)-g_1(y-\langle x\rangle)-ig_2\}\langle x|G|y\rangle\Big]\Big|_{y=x}dx - \hbar^2 g_2^2\\
&= -\hbar^2\left[-2g+g_2^2+\int_{-\infty}^{\infty}\{-(2g+g_1)(x-\langle x\rangle)-ig_2\}^2\langle x|G|x\rangle dx\right]\\
&= -\hbar^2\left[-2g+g_2^2+\frac{(2g+g_1)^2}{2(2g_R+g_1)}-g_2^2\right] = \hbar^2\left[g_R-\frac{1}{2}g_1+\frac{2g_I^2}{2g_R+g_1}\right],\\
\sigma^{(11)} &= \frac{1}{2}\langle xp+px\rangle - \langle x\rangle\langle p\rangle = \frac{\hbar}{i}\int_{-\infty}^{\infty}\left[\frac{1}{2}+x\frac{\partial}{\partial x}\right]\langle x|G|y\rangle\Big|_{y=x}dx + \hbar g_2\langle x\rangle\\
&= \frac{\hbar}{2i}+\hbar g_2\langle x\rangle + \frac{\hbar}{i}\int_{-\infty}^{\infty}x[-2g(x-\langle x\rangle)-g_1(y-\langle x\rangle)-ig_2]\langle x|G|y\rangle\Big|_{y=x}dx\\
&= \frac{\hbar}{2i}+\hbar g_2\langle x\rangle - \frac{\hbar(2g+g_1)}{2i(2g_R+g_1)} - \hbar g_2\langle x\rangle = -\frac{\hbar g_I}{2g_R+g_1} = -2\hbar g_I\sigma^{(20)}.
\end{aligned} \tag{2.5}$$

In the momentum moment calculations, it is indicated how all the position derivatives are to be calculated before setting $y = x$ and then doing the position integral.

These equations can be used to evaluate the "$g$" coefficients but it is more useful to first look at the square of the covariance-free uncertainty, Eq (1.19),

$$\begin{aligned}
M \equiv U^2 = \sigma^{(20)}\sigma^{(02)} - [\sigma^{(11)}]^2 &= \frac{2g_R-g_1}{2g_R+g_1}\frac{\hbar^2}{4} = \frac{\hbar^2}{2}(2g_R-g_1)\sigma^{(20)}\\
&= \frac{\hbar^2}{2}(2g_R+g_1-2g_1)\sigma^{(20)} = \frac{\hbar^2}{4}-\hbar^2\sigma^{(20)}g_1.
\end{aligned} \tag{2.6}$$

This identifies $g_1$ as

$$g_1 = \frac{\hbar^2/4 - M}{\hbar^2\sigma^{(20)}}, \tag{2.7}$$

from which one of the previous identities gives

$$g_R = \frac{\hbar^2/4 + M}{2\hbar^2\sigma^{(20)}}. \tag{2.8}$$

From Eq (2.5) the other two coefficients are

$$g_I = -\frac{\sigma^{(11)}}{2\hbar\sigma^{(20)}} \quad \text{and} \quad g_2 = -\frac{\langle p\rangle}{\hbar}. \tag{2.9}$$

Thus the complex coefficient is given in terms of the moments as

$$g = \frac{\hbar^2/4 + M - i\hbar\sigma^{(11)}}{2\hbar^2\sigma^{(20)}}. \tag{2.10}$$

The position representation of the gaussian operator then has the form

$$\begin{aligned}\langle x|G|y\rangle \;=\; & \frac{1}{\sqrt{2\pi\sigma^{(20)}}}\exp\Bigg[-\frac{\hbar^2/4 + M - i\hbar\sigma^{(11)}}{2\hbar^2\sigma^{(20)}}(x-\langle x\rangle)^2 - \frac{\hbar^2/4 + M + i\hbar\sigma^{(11)}}{2\hbar^2\sigma^{(20)}}(y-\langle x\rangle)^2 \\ & -\frac{\hbar^2/4 - M}{\hbar^2\sigma^{(20)}}(x-\langle x\rangle)(y-\langle x\rangle) + i\frac{\langle p\rangle}{\hbar}(x-y)\Bigg].\end{aligned} \tag{2.11}$$

For $G$ to be a density operator, at least the Schrödinger- Robertson uncertainty, equivalently $U \geq \hbar/2$, should be satisfied. However, fundamentally, $G$ must be a positive operator. That this is satisfied if $U \geq \hbar/2$ is proven in Section 3 by finding the eigenvalues of $G$ and showing that this condition is sufficient to show that all eigenvalues are positive. If this condition is not satisfied, then $G$ is not a density operator but could be a quantum operator with some other meaning, just not a density operator. The remainder of this section assumes that this condition is satisfied so that $G$ is replaced by $\rho$ to designate that the gaussian operator is now a density operator.

It is noticed that if $g_1 = 0$ in Eq (2.1), then the gaussian factors, namely

$$\langle x|\rho|y\rangle = \chi(x)\chi^*(y), \tag{2.12}$$

indicate that now $\rho$ is a pure state with wavefunction

$$\chi(x) = \frac{e^{i\phi}}{(2\pi\sigma^{(20)})^{1/4}}\exp[-g(x-\langle x\rangle)^2 + ig_2(x-\langle x\rangle)]. \tag{2.13}$$

An arbitrary phase factor $e^{i\phi}$ has been inserted, the normalization constant of $\rho$ factored between $\chi(x)$ and $\chi^*(y)$ and a term proportional to $\langle x\rangle$ inserted in each to retain the $x$ dependence of $\chi(x)$ to be of the form $x - \langle x\rangle$. The inserted terms are phase factors so cancel out between $\chi(x)$ and $\chi^*(y)$. Since the factorization requires $g_1 = 0$, equivalently $M = \hbar^2/4$ and thus $U = \hbar/2$, this means that the covariant-free uncertainty is a minimum for a quantum gaussian density operator and such a density operator is a pure state (the density operator associated with a wavefunction). Another way of classifying this is to say that the Schrödinger-Robertson uncertainty relation is an equality, equivalently that the covariance-free uncertainty is $\hbar/2$.

Using the particular value of $M$ that allows factorization,

$$g = \frac{1 - 2i\sigma^{(11)}/\hbar}{4\sigma^{(20)}} \quad \text{and} \quad g_2 = -\langle p\rangle/\hbar, \tag{2.14}$$

so the main position dependence of $\chi(x)$ not only is gaussian but has oscillations of both the quadratic and the linear term in $x$. If the covariance vanishes, then the position dependence has a gaussian form with oscillations associated with the mean momentum, namely

$$\chi(x) = \frac{e^{i\phi}}{(2\pi\sigma^{(20)})^{1/4}} \exp\left[-\frac{(x-\langle x\rangle)^2}{4\sigma^{(20)}} + i\frac{\langle p\rangle(x-\langle x\rangle)}{\hbar}\right]. \tag{2.15}$$

This is known as a coherent state and satisfies the minimum Heisenberg uncertainty $\sigma_x\sigma_p = \hbar/2$ because it has no position-momentum covariance.

### *2.1. Phase space equivalence*

For translational degrees of freedom, an operator can be represented by a function in phase space [8, 10] and arose in early quantum theory when finding the operator equivalent to a phase space observable [8] and, conversely, the definition of the Wigner function as the phase space representation of the density operator [10]. This is mentioned here since the phase space function is best expressed with coefficients expressed in terms of the moments, and connects with the classical equivalence of the free motion of a gaussian density operator described in Section 4.

For 1-dimension, the phase space function $f(x, p)$ for an operator $A$ expressed in position representation is obtained by the Fourier transform

$$f(x,p) = \frac{1}{h}\int_{-\infty}^{\infty} e^{-ipX/\hbar}\langle x + X/2|A|x - X/2\rangle dX. \tag{2.16}$$

Essentially, the phase space position $x$ is the average of the bra and ket positions of the operator, while the phase space momentum is the Fourier transform of the difference. In the present case, the operator is the gaussian $G$ with position representation given by Eq (2.1), thus squaring the terms of the independent variables $x$ and $X$,

$$f(x,p) = \frac{N}{h}\int_{-\infty}^{\infty} \exp\left[-(2g_R+g_1)(x-\langle x\rangle)^2 - \frac{(2g_R-g_1)}{4}(X-X_0)^2 + \frac{(2g_R-g_1)}{4}X_0^2\right]dX \tag{2.17}$$

where

$$X_0 = \frac{-2i}{2g_R-g_1}\left[2g_I(x-\langle x\rangle) + g_2 + \frac{p}{\hbar}\right]. \tag{2.18}$$

On carrying out the $X$ integral and grouping the various terms

$$\begin{aligned} f(x,p) &= \frac{2N}{h}\sqrt{\frac{\pi}{2g_R-g_1}}\exp\left[-\left(2g_R+g_1+\frac{4g_I^2}{2g_R-g_1}\right)(x-\langle x\rangle)^2\right. \\ &\qquad \left. -\frac{(g_2+p/\hbar)^2 + 4g_I(g_2+p/\hbar)(x-\langle x\rangle)}{2g_R-g_1}\right] \\ &= \frac{1}{2\pi\sqrt{M}}\exp\left[\frac{-\sigma^{(02)}(x-\langle x\rangle)^2 - \sigma^{(20)}(p-\langle p\rangle)^2 + 2\sigma^{(11)}(x-\langle x\rangle)(p-\langle p\rangle)}{2M}\right], \end{aligned} \tag{2.19}$$

where the last form has put in the values of the "$g$" s in terms of the moments. This could also be derived by starting with an arbitrary phase space gaussian and then evaluating the various constants

in terms of the moments, similar to the derivation of Eq (2.11) from Eq (2.1). Essentially, this means by a purely classical method. Thus, if $\hbar$ is set to 0, the expectation arguments of Section 1.2 are still valid, requiring $M \geq 0$ rather than $\hbar^2/4$. As mentioned earlier, if $M \geq \hbar^2/4$, then the gaussian, whether written in position representation or as a phase space function has a quantum interpretation as representing a density operator, but if $\hbar^2/4 > M > 0$, then the gaussian cannot be a density operator but could represent some other quantum operator. On the other hand, as long as $M > 0$, Eq (2.19) is a valid classical distribution function, including the case $M \geq \hbar^2/4$, so that classical and quantum results are the same in the latter case.

## 3. Eigenvalues and eigenvectors for a hermitian gaussian operator

The method used here was motivated by the analogous problem of finding the eigenvalues and eigenvectors for the gaussian Keilson-Storer collision kernel [17]. That was done for both 1 and 3-dimensional variables.

Since the operator is a gaussian, it is reasonable to assume that at least one of the eigenvectors is a gaussian. For convenience in writing, $\langle x \rangle$ is set equal to 0 in this section, equivalently that $x$ is shorthand for $x - \langle x \rangle$. Thus, write

$$\chi_0(x) = \exp(-c_2 x^2 - c_1 x - c_0) \tag{3.1}$$

with unknown constants $c_2, c_1, c_0$. If this is an eigenvector of $G$, then it should satisfy

$$\lambda_0 \chi_0(x) = \int_{-\infty}^{\infty} \langle x|G|y\rangle \chi_0(y) dy, \tag{3.2}$$

with its eigenvalue $\lambda_0$. The integral in this equation is evaluated according to

$$\begin{aligned}
\int_{-\infty}^{\infty} \langle x|G|y\rangle \chi_0(y) dy &= \frac{1}{\sqrt{2\pi\sigma^{(20)}}} \exp\left[-gx^2 - ig_2 x - c_0\right] \int_{-\infty}^{\infty} \exp\left[-g^* y^2 - g_1 xy + ig_2 y - c_2 y^2 - c_1 y\right] dy \\
&= \frac{1}{\sqrt{2\pi\sigma^{(20)}}} \exp\left[-gx^2 - ig_2 x - c_0\right] \int_{-\infty}^{\infty} \exp\left[-(g^* + c_2)\left(y + \frac{A}{2(g^* + c_2)}\right)^2\right] dy \exp \frac{A^2}{4(g^* + c_2)} \\
&= \frac{1}{\sqrt{2\pi\sigma^{(20)}}} \exp\left[-gx^2 - ig_2 x - c_0\right] \sqrt{\frac{\pi}{|g^* + c_2|}} \exp \frac{A^2}{4(g^* + c_2)},
\end{aligned} \tag{3.3}$$

where

$$A = g_1 x + c_1 - ig_2. \tag{3.4}$$

The integral should be equal to $\lambda_0 \exp[-c_2 x^2 - c_1 x - c_0]$, so by equating terms in the exponent, the equality of the coefficients of $x^2$ implies

$$-c_2 = -g + \frac{g_1^2}{4(g^* + c_2)} \tag{3.5}$$

and of the $x$ coefficients implies

$$-c_1 = -ig_2 + g_1 \frac{c_1 - ig_2}{2(g^* + c_2)} \tag{3.6}$$

while the equality of the constants imply the equality

$$\lambda_0 e^{-c_0} = \frac{e^{-c_0}}{\sqrt{2\sigma^{(20)}|g^* + c_2|}} \exp\left[\frac{(c_1 - ig_2)^2}{4(g^* + c_2)}\right]. \tag{3.7}$$

The equation for $c_2$ is equivalent to

$$c_2^2 + (g^* - g)c_2 = c_2^2 + \frac{i\sigma^{(11)}}{\hbar\sigma^{(20)}}c_2 = gg^* - \frac{g_1^2}{4} = \frac{\sigma^{(02)}}{4\hbar^2\sigma^{(20)}}. \tag{3.8}$$

Completing the square of the first term gives

$$\left(c_2 + \frac{i\sigma^{(11)}}{2\hbar\sigma^{(20)}}\right)^2 = \frac{\sigma^{(02)}}{4\hbar^2\sigma^{(20)}} - \frac{(\sigma^{(11)})^2}{4\hbar^2(\sigma^{(20)})^2} = \frac{M}{4\hbar^2(\sigma^{(20)})^2}. \tag{3.9}$$

There are two roots to this equation

$$c_2 = \frac{\pm\sqrt{M} - i\sigma^{(11)}}{2\hbar\sigma^{(20)}} = \frac{\pm U - i\sigma^{(11)}}{2\hbar\sigma^{(20)}}. \tag{3.10}$$

The $-$ choice is unphysical since it leads to an infinite norm for $\chi_0$. Thus it is only the root with $+U$ that is allowed. The important combination $g^* + c_2$ is

$$g^* + c_2 = \frac{U^2 + \hbar^2/4 + \hbar U}{2\hbar^2\sigma^{(20)}} = \frac{(U + \hbar/2)^2}{2\hbar^2\sigma^{(20)}}. \tag{3.11}$$

It is noticed that this is real and positive. The equation for $c_1$ clearly implies that

$$c_1 = ig_2 = -i\langle p\rangle/\hbar. \tag{3.12}$$

This simplifies the equation for the eigenvalue $\lambda_0$ so that $c_0$ is arbitrary (suitably chosen to normalize and add an arbitrary constant phase factor to $\chi_0$). The eigenvalue is

$$\lambda_0 = \frac{1}{\sqrt{2\sigma^{(20}|g^* + c_2|}} = \frac{\hbar}{U + \hbar/2}. \tag{3.13}$$

For the special case that $U = \hbar/2$, then $\lambda_0 = 1$ and $\chi_0(x) \propto \chi(x)$, Eq (2.13), the pure state into which $\rho$ factors. Thus this makes connection to the general discussion of the gaussian given in Eqs (2.12)–(2.15).

For general $U$, the gaussian eigenvector is [Note $x$ is short for $x - \langle x\rangle$ in this section.]

$$\chi_0(x) = e^{i\phi}\left[\frac{U}{\pi\hbar\sigma^{(20)}}\right]^{1/4} \exp\left[-\frac{U - i\sigma^{(11)}}{2\hbar\sigma^{(20)}}x^2 + \frac{i\langle p\rangle x}{\hbar}\right] \tag{3.14}$$

where $-c_0$ has been replaced by $i\phi$ to allow for an arbitrary phase factor of the wavefunction and the normalization has been chosen as $\int |\chi_0(x)|^2 dx = 1$.

Since the operator is a gaussian with one eienvector a gaussian, it is reasonable to assume that the other eigenvectors should involve Hermite polynomials $H_n$ as the Hermites are generated by a gaussian.

That that is the case is proven by introducing the generating function for the Hermite polynomials [18, 19]

$$e^{2\alpha xz-z^2} = \sum_{n=0}^{\infty} H_n(\alpha x)\frac{z^n}{n!}. \tag{3.15}$$

This is done with $\chi_0(x)$ acting as the gaussian weight function for the orthogonalization of the Hermite polynomials. Thus the generating function for the eigenvectors $X_n(x)$ of $\langle x|G|y\rangle$ is expected to be

$$\mathsf{G}(x,z) = e^{2\alpha xz-z^2}\chi_0(x) = \sum_{n=0}^{\infty} X_n(x)\frac{z^n}{n!} \tag{3.16}$$

with a suitably chosen $\alpha$. The orthogonality and normalization of the $X_n(x)$ follow from

$$\begin{aligned}\int_{-\infty}^{\infty}\mathsf{G}^*(x,z)\mathsf{G}(x,s)dx &= \int_{-\infty}^{\infty} e^{2\alpha x(z+s)-z^2-s^2}|\chi_0(x)|^2dx = \sqrt{\frac{U}{\pi\hbar\sigma^{(20)}}}e^{-z^2-s^2}\int_{-\infty}^{\infty}\exp\left(2\alpha x(z+s)-\frac{Ux^2}{\hbar\sigma^{(20)}}\right)dx \\ &= \exp\left(-z^2-s^2+\frac{\alpha^2\hbar\sigma^{(20)}}{U}(z+s)^2\right) = e^{2zs} = \sum_n\frac{(2zs)^n}{n!} = \sum_{n,m}\frac{z^n s^m}{n!m!}\int_{-\infty}^{\infty}X_n^*(x)X_m(x)dx, \end{aligned}\tag{3.17}$$

which implies

$$\int_{-\infty}^{\infty}X_n^*(x)X_m(x)dx = 2^n n!\delta_{nm}. \tag{3.18}$$

In the above, the exponent was organized to complete the square in $x$, after which the $x$ integration was straightforward. It was then required to set $\alpha^2 = U/\hbar\sigma^{(20)}$ in order to simplify the expression in terms of $zs$, thus identifying a proper choice for $\alpha$ in order to make the eigenvectors orthogonal. The normalization of Eq (3.18) is natural for the generating function but inappropriate for expressing the spectral properties of an operator, (compare Section 1.1) so the renormalized set of eigenvectors

$$\chi_n(x) \equiv \frac{1}{\sqrt{2^n n!}}X_n(x) \tag{3.19}$$

is introduced for later use.

Provided the $X_n(x)$ are eigenvectors of the gaussian $G$, the action of $G$ on the generator $\mathsf{G}$ should reproduce the eigenvectors together with their eigenvalues. To see that this works out, the above action is formally

$$\mathsf{G}_1(x,z) \equiv \int_{-\infty}^{\infty}\langle x|G|y\rangle\mathsf{G}(y,z)dy \tag{3.20}$$

and the detailed form of the resulting generator $\mathsf{G}_1$ examined. Carrying out the integral gives

$$\begin{aligned}\mathsf{G}_1(x,z) &= \frac{e^{-gx^2-ig_2x}}{\sqrt{2\pi\sigma^{(20)}}}\int_{-\infty}^{\infty}e^{-g^*y^2-g_1xy+ig_2y+2\alpha yz-z^2}\chi_0(y)dy \\ &= \frac{e^{-gx^2-ig_2x-z^2+i\phi}}{\sqrt{2\pi\sigma^{(20)}}}\left[\frac{U}{\pi\hbar\sigma^{(20)}}\right]^{1/4}\int_{-\infty}^{\infty}e^{-B(y-D/2B)^2}dy\, e^{D^2/4B} = \frac{e^{-gx^2-ig_2x-z^2+i\phi}}{\sqrt{2\sigma^{(20)}B}}\left[\frac{U}{\pi\hbar\sigma^{(20)}}\right]^{1/4}e^{D^2/4B}, \end{aligned}\tag{3.21}$$

where

$$B = g^* + \frac{U-i\sigma^{(11)}}{2\hbar\sigma^{(20)}} = \frac{(U+\hbar/2)^2}{2\hbar^2\sigma^{(20)}} \tag{3.22}$$

is the same as $g^* + c_2$, Eq (3.11), and $D = -g_1 x + 2\alpha z$. The exponent that appears in $\mathsf{G}_1$ is

$$\begin{aligned} & -gx^2 - ig_2 x - z^2 + i\phi + \frac{2\hbar^2\sigma^{(20)}}{(U+\hbar/2)^2}\left(\frac{g_1^2 x^2}{4} - g_1\alpha z x + \alpha^2 z^2\right) \\ = \; & -\frac{U - i\sigma^{(11)}}{2\hbar\sigma^{(20)}}x^2 + \left[\frac{i\langle p\rangle}{\hbar} + 2\frac{(U-\hbar/2)}{U+\hbar/2}\alpha z\right]x + \frac{(U-\hbar/2)^2}{(U+\hbar/2)^2}z^2 + i\phi. \end{aligned} \tag{3.23}$$

It is seen that the $z$ independent terms are what appear in the exponent of $\chi_0(x)$ while the $z$ dependent terms are what appear in the Hermite polynomial generating function except that $z$ is multiplied by the factor

$$\frac{U-\hbar/2}{U+\hbar/2} \equiv \gamma. \tag{3.24}$$

Furthermore, the prefactor in front of the exponent appears different. Thus it appears that $\mathsf{G}_1(x,z)$ has the structure $N'\mathsf{G}(x,\gamma z)$, in terms of a scaled version of Eq (3.16). Since the $[\cdots]^{1/4}$ factor appears in $\chi_0(x)$, the prefactor $N'$ in $\mathsf{G}_1(x,z)$ is

$$N' = \frac{1}{\sqrt{2\sigma^{(20)}B}} = \frac{\hbar}{U+\hbar/2}. \tag{3.25}$$

Now expand the generating function equality, namely

$$N'\mathsf{G}(x,\gamma z) = \int_{-\infty}^{\infty}\langle x|G|y\rangle\mathsf{G}(y,z)dy \tag{3.26}$$

in powers of $z$, which shows that

$$N'\gamma^n X_n(x) = \int_{-\infty}^{\infty}\langle x|G|y\rangle X_n(y)dy \tag{3.27}$$

and thus that

$$X_n(x) = H_n(\alpha x)\chi_0(x) \tag{3.28}$$

is an eigenvector of $G$ with eigenvalue

$$\lambda_n = N'\gamma^n = \frac{\hbar}{U+\hbar/2}\left(\frac{U-\hbar/2}{U+\hbar/2}\right)^n. \tag{3.29}$$

This also includes $n = 0$ since $H_0(\alpha x) = 1$. These eigenvalues sum to 1, namely

$$\sum_{n=0}^{\infty}\lambda_n = \frac{\hbar}{U+\hbar/2}\sum_{n=0}^{\infty}\gamma^n = \frac{\hbar}{U+\hbar/2}\frac{1}{1-\gamma} = 1, \tag{3.30}$$

which is consistent with $\mathrm{Tr}G = \iint f(x,p)dxdp = 1$. This verifies that all eigenvalues have been found. Note that the $X_n$ are normalized according to Eq (3.18). Renormalizing them according to Eq (3.19), the spectral representation of $G$ can be written

$$\langle x|G|y\rangle = \sum_{n=0}^{\infty}\langle x|\chi_n\rangle\lambda_n\langle\chi_n|y\rangle = \sum_{n=0}^{\infty}\chi_n(x)\lambda_n\chi_n^*(y). \tag{3.31}$$

These results are valid for arbitrary $U > 0$. If $U < \hbar/2$, then $\gamma < 0$ and the eigenvalues $\lambda_n$ alternate in sign as $n$ varies. Clearly not all eigenvalues are positive so $G$ cannot be a density operator, but could represent some other quantum operator. Provided $U > \hbar/2$ then all eigenvalues are positive and $G$ could be interpreted as a mixed state density operator with an infinite number of eigenfunctions $\chi_n(x)$. As $U \to \hbar/2$ all eigenvalues approach 0 except for $\lambda_0 \to 1$, and $G$ approaches the pure state density operator associated with wavefunction $\chi_0(x)$.

## 4. Free motion time dependence of a gaussian operator

This is a classic topic in quantum mechanics in that the free motion of a gaussian wave packet spreads out with time, see e.g., [20]. Gaussian wave functions have been used to computationally model the motion of a wave packet. In particular, the penetration of a 1-dimensional barrier was first discussed by Heller [21] using classical mechanics to determine the time dependence of the coefficients in the wave packet. The present author [22] emphasized an approximation of the quantum time dependence of the position and momentum moments to determine the time dependence of the coefficients of a gaussian pure state density matrix. Actually, it was an earlier examination [16] of a moment method for classical and quantal dynamics that drew the authors attention to what is here called the covariance-free uncertainty, but unfamiliarity with the Schrödinger- Robertson uncertainty relation and the lack of knowing how to determine whether a gaussian operator was a density operator necessitated using pure states for the barrier penetration mentioned earlier.

Here it is only the free motion time dependence that is discussed and it is shown that a negative value for the covariance can lead to non-intuitive time dependence. This was recently discovered for pure states and short times after starting the motion by detailed computation [12, 13], but is shown here to also occur at very large times, depending on the relative values of the initial moments. It is also shown that these properties can arise for mixed gaussian states as well as for classical gaussian distribution functions.

Free motion is governed in time $t$ by the kinetic hamiltonian $H = p^2/2m$, either classically via Newton's equations

$$\frac{dx}{dt} = \frac{\partial H}{\partial p} = \frac{p}{m} \quad \text{and} \quad \frac{dp}{dt} = \frac{\partial H}{\partial x} = 0 \tag{4.1}$$

or quantum mechanically [using the Heisenberg picture]

$$\frac{dx}{dt} = \frac{i}{\hbar}[Hx - xH] = \frac{p}{m} \quad \text{and} \quad \frac{dp}{dt} = \frac{i}{\hbar}[Hp - pH] = 0, \tag{4.2}$$

with an obvious dual use of terminology so as to avoid having to deal with any symbolism to distinguish classical variables from quantum operators and explicitly writing out the commutator in the latter case. This emphasizes the formal similarity of the equations of motion for the position and momentum observables and shows that

$$x(t) = x_o + \frac{p_o}{m}t \quad \text{and} \quad p(t) = p_o \tag{4.3}$$

with the subscript o denoting their initial ($t = 0$) values. It follows that the equations of motion for the position-momentum moments have analogous properties, namely for the pure momentum moments, these are constant with time

$$\begin{aligned} \langle p\rangle(t) &\equiv \langle p(t)\rangle = \langle p_o\rangle \equiv \langle p\rangle_o, \\ \sigma^{(02)}(t) &= \langle (p-\langle p\rangle)^2\rangle_o \equiv \sigma_o^{(02)}. \end{aligned} \tag{4.4}$$

Note that these describe properties of the time constant distribution of the momentum. The position dependent moments are

$$\langle x\rangle(t) \equiv \langle x(t)\rangle = \langle x_o + \frac{p_o}{m}t\rangle = \langle x\rangle_o + \frac{\langle p\rangle_o}{m}t, \tag{4.5}$$

$$\begin{aligned} \sigma^{(11)}(t) &= \langle [x(t)-\langle x\rangle(t)](p-\langle p\rangle)\rangle = \langle \left(x_o + \frac{p}{m}t - \langle x\rangle_o - \frac{\langle p\rangle}{m}t\right)(p-\langle p\rangle)\rangle \\ &= \langle (x_o - \langle x\rangle_o)(p-\langle p\rangle)\rangle + \langle (p-\langle p\rangle)^2\rangle_o \frac{t}{m} = \sigma_o^{(11)} + \sigma_o^{(02)}\frac{t}{m} \end{aligned} \tag{4.6}$$

and

$$\begin{aligned} \sigma^{(20)}(t) &= \langle [x(t)-\langle x\rangle(t)]^2\rangle = \langle \left[x_o + \frac{p_o}{m}t - \langle x\rangle_o - \frac{\langle p\rangle_o t}{m}\right]^2\rangle \\ &= \sigma_o^{(20)} + 2\sigma_o^{(11)}\frac{t}{m} + \sigma_o^{(02)}\frac{t^2}{m^2} = \sigma_o^{(02)}\left(\frac{t}{m} + \frac{\sigma_o^{(11)}}{\sigma_o^{(02)}}\right)^2 + \sigma_o^{(20)} - \frac{(\sigma_o^{(11)})^2}{\sigma_o^{(02)}}, \end{aligned} \tag{4.7}$$

with the last form of $\sigma^{(20)}(t)$ showing that this is positive as long as $M = U^2 > 0$, which is also a condition for $f(x,p)$, Eq (2.19), to have any meaning, even classically. It is noted that, as used in this section, these relations use the gaussian density operator Eq (2.11), and/or its phase space equivalent, Eq (2.19) for evaluating all the expectation values. In effect this is taken as the initial state for the time evolution where its parameters could be listed with subscript o to emphasise that these are the initial values of the parameters (expectation values). In quantum mechanics, this is the Heisenberg picture of time evolution.

The Schrödinger picture leaves the observables constant and has the density operator evolving with time. Because of the simple relation between the gaussian density operator and its expectation values (moments), the time dependent density operator is just Eq (2.11) with the time dependent moments replacing the initial moments. Such a result could also be obtained by solving the quantum Liouville equation [also called the von Neumann equation] for the time evolution, equivalently the Liouville equation in the classical case. But the simplicity of the gaussian is that the gaussian stays a gaussian during free motion, both classically and quantum mechanically, just the values of the coefficients change.

Since the momentum moments are constant in free motion, the description of the evolution is all in the position dependence and needs only the position distribution function $F(x,t)$, both classically and also quantum mechanically since this is a diagonal part of the density matrix. This is obtained as

$$\begin{aligned} F(x,t) &= \langle x|G(t)|x\rangle = \int f(x,p,t)dp \\ &= \frac{1}{\sqrt{2\pi\sigma^{(20)}(t)}}\exp\left[-\frac{(x-\langle x\rangle(t))^2}{2\sigma^{(20)}(t)}\right]. \end{aligned} \tag{4.8}$$

Note that a $t$ dependence has been added to $G$ and $f$ to indicate that the coefficients are now time dependent according to Eqs (4.5)–(4.7). To connect with [12, 13], the initial mean position $\langle x\rangle_o < 0$ and momentum $\langle p\rangle_o > 0$ are set so that the packet described by Eq (4.8) is expected to move from a negative to a positive position on the basis of the mean position and momentum. To monitor what happens, the fraction of the packet in the positive $x$ half space is

$$F_+(t) \equiv \int_0^\infty F(x,t)dx = \frac{1}{\sqrt{\pi}}\int_{z(t)}^\infty e^{-u^2}du = \frac{1}{2}\text{erfc}[z(t)] \tag{4.9}$$

where erfc is the complementary error function,

$$u \equiv \frac{x-\langle x\rangle(t)}{\sqrt{2\sigma^{(20)}(t)}} \quad \text{and} \quad z(t) \equiv \frac{-\langle x\rangle(t)}{\sqrt{2\sigma^{(20)}(t)}}. \tag{4.10}$$

$z(t)$ varies with time from its initial value at $t = 0$ to its final value at $t = \infty$ according to

$$z(0) = \frac{-\langle x\rangle_o}{\sqrt{2\sigma_o^{(20)}}} \quad \text{to} \quad z(\infty) = \frac{-\langle p\rangle_o}{\sqrt{2\sigma_o^{(02)}}}. \tag{4.11}$$

Note that the time dependence of $\langle x\rangle(t)$ and $\sqrt{\sigma^{(20)}(t)}$ cancel out at large times and that the initial and final $z$ and consequently $F_+$ values bear no relation to each other. It is also noted that $z(0) > 0$ and $z(\infty) < 0$ so that $F_+(0)$ is less than $F_+(\infty)$ and there is a net accumulation of particles in the positive half space as would be expected from the center of the packet moving to the right. These results follow from the formalism but their rationalization depends on remembering that it is the packet that moves, not the position in the packet that is used to divide the packet into what region is chosen to monitor. The latter position has been chosen here as $x = 0$ whereas in [12] and [13] this was chosen as an arbitrary $q$ and adds another parameter, which is unecessary in this author's opinion.

Since erfc($z$) decreases with increasing $z$, it is useful to examine how $-z(t)$ varies since this defines how $F_+(t)$ increases. Using the detailed time dependence of the moments, this is

$$-z(t) = \frac{\langle x\rangle_o + \langle p\rangle_o t/m}{\sqrt{2\sigma_o^{(20)} + 4\sigma_o^{(11)}t/m + 2\sigma_o^{(02)}t^2/m^2}}. \tag{4.12}$$

Its rate of change reflects the rate of change of $F_+(t)$ and is

$$-\frac{dz(t)}{dt} = \frac{2}{m[2\sigma_o^{(20)}(t)]^{3/2}}\left[\langle p\rangle_o\sigma_o^{(20)} - \langle x\rangle_o\sigma_o^{(11)} + (\langle p\rangle_o\sigma_o^{(11)} - \langle x\rangle_o\sigma_o^{(02)})\frac{t}{m}\right] \tag{4.13}$$

Note that $\langle x\rangle_o < 0$, $\langle p\rangle_o > 0$ and $t \geq 0$ so the only quantity in the rate equation that can vary in sign is $\sigma_o^{(11)}$. Clearly, if $\sigma_o^{(11)} \geq 0$ then the rate of change is always positive as might be intuitively considered, while if negative a variation in behavior occurs.

### *4.1. Rate of change of $F_+(t)$ when $\sigma_o^{(11)} < 0$*

At initial and small times the sign of the rate is determined by the combination $\langle p\rangle_o\sigma_o^{(20)} - \langle x\rangle_o\sigma_o^{(11)}$, so the rate is positive if

$$\langle x\rangle_o\sigma_o^{(11)} < \langle p\rangle_o\sigma_o^{(20)} \tag{4.14}$$

and negative if the opposite inequality is valid. Note that both terms that are being compared are positive. Effectively, if $\sigma_o^{(11)}$ has a small negative value, then $F_+(t)$ increases with time just as it would if $\sigma_o^{(11)}$ was positive. $F_+(t)$ decreases only if $\sigma_o^{(11)}$ is sufficiently negative, namely

$$-\sigma_o^{(11)} > \frac{\langle p\rangle_o \sigma_o^{(20)}}{-\langle x\rangle_o}. \tag{4.15}$$

This is the case that was discovered in [12] and [13] and reflects how the packet spread decreases at a rate fast enough so the translation of the packet cannot increase $F_+(t)$.

At sufficiently large times the second term in Eq (4.13) will dominate so that $F_+(t)$ increases with time if

$$-\langle p\rangle_o \sigma_o^{(11)} < -\langle x\rangle_o \sigma_o^{(02)} \tag{4.16}$$

and decreases with the opposite inequality. Note that the negative signs in this inequality have been introduced so that each term is positive. Effectively this requires $-\sigma_o^{(11)}$ to be small for increasing $F_+(t)$ while for decreasing $F_+(t)$ it must be sufficiently large, namely

$$-\sigma_o^{(11)} > \frac{-\langle x\rangle_o \sigma_o^{(02)}}{\langle p\rangle_o}. \tag{4.17}$$

An alternate and possibly clearer way of understanding this result is to expand the dependence of $-z(t)$ in powers of $1/t$, thus

$$\begin{aligned} -z(t) &= \frac{\langle p\rangle_o + \langle x\rangle_o m/t}{\sqrt{2\sigma_o^{(02)} + 4\sigma_o^{(11)} m/t + 2\sigma_o^{(20)} m^2/t^2}} \\ &= \frac{\langle p\rangle_o}{\sqrt{2\sigma_o^{(02)}}}\left[1 + \left(\frac{\langle x\rangle_o}{\langle p\rangle_o} - \frac{\sigma_o^{(11)}}{\sigma_o^{(02)}}\right)\frac{m}{t} + O\left(\frac{m^2}{t^2}\right)\right]. \end{aligned} \tag{4.18}$$

If Eq (4.17) is satisfied the $(\cdots)$ bracket is positive so that as $t$ increases, $1/t$ decreases and so does $-z(t)$ and $F_+(t)$. This large time case was not considered in [12] or [13], presumably because neither considered the asymptotic (large time) behavior.

Note that the conditions (4.15), (4.17) are different though both require $-\sigma_o^{(11)}$ to be large for decreasing $F_+(t)$. Decreasing $F_+(t)$ for both cases cannot occur for the same set of moments because the product of the inequalities,

$$\left[\sigma_o^{(11)}\right]^2 > \sigma_o^{(20)}\sigma^{(02)} \tag{4.19}$$

violates the normalization condition $M > 0$ of the phase space gaussian, Eq (2.19), which is required both classically and quantally. This is consistent with the earlier comment that $F_+(\infty) > F_+(0)$ associated with the final and initial values of $z(t)$. That is, there is always a net increase in $F_+$ and any period of time during which $F_+(t)$ may decrease is a transient effect.

## 5. Discussion

An arbitrary normalized gaussian operator is rewritten with its independent parameters expressed as functions of the position and momentum moments. The phase space equivalent, obtained by the

Wigner-Weyl transformations, is also a gaussian expressed in terms of the same parameters. From the review of density operators, Section 1.1, for an operator to be density operator, all its eigenvalues must be positive. The condition that this is the case for a gaussian operator is shown in Section 3 to be that the Schrödinger-Robertson uncertainty (equivalently $U \geq \hbar/2$) is satisfied. This result is presumably new. Thus, gaussian operators are classified as to whether they cannot, $U < \hbar/2$, or can, $U \geq \hbar/2$, be considered a density operator. The equality implies that it can represent a pure state, whereas inequality implies it can represent a mixed state with eigenvalues that are functions of $U$, see Section 3. The corresponding eigenvectors are Hermite polynomials of a scaled position times a particular gaussian weighting factor. As a related problem, the free motion evolution of a gaussian operator, equivalently phase space function, has been classified as to whether the amount of the packet in the positive half space as it moves forward continuously increases or whether there are periods of time when it decreases. It is found that the latter can occur if the position-momentum covariance is sufficiently negative, either at small or large times. This classification is valid whether the state obeys classical or quantum mechanics and either a pure or mixed state in the latter case. Previous treatments of such an evolution has been considered only for pure states and often with no position-momentum covariance.

## Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

## Conflict of interest

The author declares there is no conflict of interest.

## References


1. I. N. Levine, *Quantum Chemistry,7e*, Pearson, (2016).
2. P. R. Kaprálová-Žďánská, J. Šmydke, Gaussian basis sets for highly excited and resonance states of helium, *J. Chem. Phys.*, **138** (2013), 024105. https://doi.org/10.1063/1.4772468
3. M. Sargent III, M. O. Scully, W. E. Lamb Jr., *Laser Physics*, Addison-Wesley, (1974).
4. E. Schrödinger, About Heisenberg uncertainty relation, *arXiv preprint*, (1999), arXiv:quant-ph/9903100. https://doi.org/10.48550/arXiv.quant-ph/9903100
5. H. P. Robertson, The uncertainty principle, *Phys. Rev.*, **34** (1929), 163. https://doi.org/10.1103/PhysRev.34.163
6. K. Gottfried, *Quantum Mechanics: Fundamentals*, CRC Press, (2018). https://doi.org/10.4324/9780429493225
7. D. A. Trifonov, Schrödinger uncertainty relation and its minimization states, *arXiv preprint*, (2001), arXiv:physics/0105035. https://doi.org/10.48550/arXiv.physics/0105035
8. H. Weyl, *The Theory of Groups and Quantum Mechanics*, Courier Corporation, (1950).
9. W. B. Case, Wigner functions and Weyl transforms for pedestrians, *Amer. J. Phys.*, **76** (2008), 937–946. https://doi.org/10.1119/1.2957889

10. E. Wigner, On the quantum correction for thermodynamic equilibrium, *Phys. Rev.*, **40** (1932), 749. https://doi.org/10.1103/PhysRev.40.749
11. U. Fano, Description of states in quantum mechanics by density matrix and operator techniques, *Rev. Mod. Phys.*, **29** (1957), 74. https://doi.org/10.1103/RevModPhys.29.74
12. A. A. D. Villanneva, The negative flow of probability, *Am. J. Phys.*, **88** (2020), 325–333. https://doi.org/10.1119/10.0000856
13. A. Goussev, Comment on "The negative flow of probability", *Am. J. Phys.*, **88** (2020), 1023–1028. https://doi.org/10.1119/10.0001773
14. J. von Neumann, *Mathematical Foundations of Quantum Mechanics*, Princeton university press, (2018).
15. R. Schatten, *Norm Ideals of Completely Continuous Operators*, Springer-Verlag, (2013).
16. R. E. Turner, R. F. Snider, A phase space moment method for classical and quantal dynamics, *Can. J. Phys.*, **59** (1981), 457–470. https://doi.org/10.1139/p81-057
17. R. F. Snider, Eigenvectors and eigenvalues for the Keilson-Storer collision kernel, *Phys. Rev. A*, **33** (1986), 178. https://doi.org/10.1103/PhysRevA.33.178
18. M. Abramowitz, I. A. Stegun, *Handbook of Mathematical Functions*, Dover, New York, (1968).
19. H. Bateman, *Higher Transcendental Functions*, McGraw-Hill, (1953).
20. L. I. Schiff, *A Textbook of Quantum Mechanics*, McGraw-Hill Book Company, (1949).
21. E. J. Heller, Time-dependent approach to semiclassical dynamics, *J. Chem. Phys.*, **62** (1975), 1544–1555. https://doi.org/10.1063/1.430620
22. R. E. Turner, R. F. Snider, A comparison of local and global single gaussian approximations to time dynamics: one dimensional systems, *J. Chem. Phys.*, **87** (1987), 910–920. https://doi.org/10.1063/1.453246


AIMS Press

© 2023 the Author(s), licensee AIMS Press. This is an open access article distributed under the terms of the Creative Commons Attribution License (http://creativecommons.org/licenses/by/4.0)