Invariant operators for quadratic Hamiltonians

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The motion of wave packets can be easily determined for any Hamiltonian that is quadratic in position and momentum, even if the coefficients of the terms in the Hamiltonian vary with time. The method is based on the existence of an invariant operator, linear in position and momentum, the coefficients of these operators being solutions of the corresponding classical system. This immediately yields a set of very simple wave packets whose evolution is easily determined, and whose magnitude has the same form as the energy eigenfunctions of the harmonic oscillator (i.e., Gaussian or Hermite–Gaussian). This set provides a complete basis for finding the evolution of any state and the exact propagator is readily determined. For the harmonic oscillator, this set includes coherent states, squeezed states, displaced number states, and squeezed number states as special cases. The following important properties hold for every quadratic Hamiltonian, no matter what time dependence is present in the Hamiltonian: (1) The motion of the centroid of any wave packet separates from that of any moments relative to the centroid. (2) Every detail of the evolution of the quantum system can be calculated from the solutions of the corresponding classical system. (3) Wave functions of Gaussian (or Hermite–Gaussian) form will retain that form as they evolve.

I. INTRODUCTION

One of the disappointments about most introductory courses on quantum mechanics is that they contain so little about the motion of wave packets. The main emphasis is on the eigenfunctions of the Hamiltonian and these have no motion if bound and are not normalisable if unbound. Historically these energy eigenfunctions were very important because of their direct application to spectroscopy, but wave packet motion is important in considering quantum mechanics as a complete theory and understanding its relation to classical mechanics. In part, the reason for the neglect of wave packet motion has been the technical difficulty of dealing with it in terms of eigenfunctions of the Hamiltonian. Here I will show that, for an important class of Hamiltonians, one can easily find endless examples of simple wave packets whose evolution is simply determined in terms of the solutions of the corresponding classical system. Furthermore, these wave packets provide a complete basis from which the motion of an arbitrary wave function can be calculated. (The term ''wave packet,'' instead of ''wave function,'' will indicate normalisability and the existence of the expectation values of position and momentum and their squares.)

A quadratic Hamiltonian is one that is quadratic in the position and momentum operators. Thus, for a Hermitian Hamiltonian in one space dimension, the most general form is

$$\hat{H}=\tfrac{1}{2}a\hat{p}^2+\tfrac{1}{2}b(\hat{p}\hat{x}+\hat{x}\hat{p})+\tfrac{1}{2}c\hat{x}^2+f\hat{p}+g\hat{x}. \tag{1}$$

The analysis used here works even when the coefficients a, b, c, f, g vary with time. These quadratic Hamiltonians include many important cases; for example: free particle; particle moving vertically under gravity; particle in a time-varying, spatially homogeneous electric field; harmonic oscillator; driven harmonic oscillator (g varying with time).

Usually $b=0$ and then $a=1/m$ and $c=m\omega^2$ (if it is positive); the mass m and frequency ω may vary with time. We keep the term $\hat{p}\hat{x}+\hat{x}\hat{p}$ in the development of the theory because it can represent a homogeneous magnetic field in more than one dimension and because an arbitrary Hamiltonian can be approximated locally by a quadratic one if the wave function is sufficiently localised.[1] This requires a time-dependent quadratic (even if the exact Hamiltonian does not vary with time) because as the system evolves the local quadratic approximation will change. In general, such an approximation will include this cross term.

There are many examples of time-dependent quadratic Hamiltonians in quantum optics, e.g., the parametric amplifier or the Paul trap. Their formulation would be in terms of creation and annihilation operators. In this paper, only the mechanical case will be considered and the formulation will be in terms of position and momentum.

The analysis used here is based on the existence of a time-dependent invariant operator. Invariant operators are generalisations of ''constants of the motion'' that allow for dependence on time. The invariant operators used here are linear in position and momentum and have the algebraic properties of oscillator raising and lowering operators. They can therefore be used to construct wave functions that, apart from a phase shift and a spatial displacement, have the same form as the energy eigenfunctions of a harmonic oscillator, i.e., a Gaussian multiplied by a Hermite polynomial (hereafter called Hermite–Gaussians). These wave functions retain this form under the Hamiltonian evolution with time.

Invariant operators, similar to those used here, were used by Lewis and Riesenfeld[2] to analyse the harmonic oscillator with time-dependent frequency. The role of these operators in constructing oscillator-like (coherent) states was investigated by Hartley and Ray.[3] Much of the present work is closely related to developments, in the context of quantum optics, of Glauber's theory of coherent states to cover displaced and squeezed number states.[4]

Very many time-dependent quadratic systems have been analysed using various methods.[2,5] One commonly used approach is based on Lie algebra.[6] The present work aims to give a simpler unified approach to this whole class of systems, an approach which emphasises their close relation with the corresponding classical systems.

Schrödinger's picture will be used throughout, but the introduction of the ''total time derivative of an operator'' will result in a great simplification in the algebra, and allow a close parallel with the classical formalism.

II. THE TOTAL TIME DERIVATIVE OF ANY OPERATOR

For any operator $\hat{A}$, its expectation value changes with time according to

$$\frac{d}{dt}\langle\hat{A}\rangle=\left\langle\frac{\partial}{\partial t}\hat{A}\right\rangle+\frac{i}{\hbar}\langle[\hat{H},\hat{A}]\rangle, \tag{2}$$

which can be found in any textbook on quantum mechanics.[7] The first term comes from the intrinsic time dependence in $\hat{A}$ and the second from the way the states change with time. It is convenient, therefore, to define the ''total time derivative'' of any operator $\hat{A}$ to be[8]

$$\frac{d}{dt}\hat{A}\equiv\dot{\hat{A}}:=\frac{\partial}{\partial t}\hat{A}+\frac{i}{\hbar}[\hat{H},\hat{A}]. \tag{3}$$

[I use $a:=b$ to denote ''a is defined to be b'']. Then it is always true that

$$\frac{d}{dt}\langle\hat{A}\rangle=\left\langle\frac{d}{dt}\hat{A}\right\rangle. \tag{4}$$

Furthermore, it can easily be seen that the definition (3) implies that

$$\frac{d}{dt}(\hat{A}\hat{B})=\dot{\hat{A}}\hat{B}+\hat{A}\dot{\hat{B}},\quad \frac{d}{dt}(f(t)\hat{A})=\dot{f}\hat{A}+f\dot{\hat{A}}, \tag{5}$$

which mean that this ''total derivative'' obeys the same algebraic rules as ordinary differentiation. It is not necessary to think of it as differentiation in the usual sense; it is enough to know that it obeys the same algebraic rules. The fact that it is not defined to be a rate of change of anything does not matter because the operator relations are never the end result; they are the means to finding wave functions, expectation values, or eigenvalues. All we ever use are the properties in Eqs. (4) and (5).

III. SOME GENERALITIES ABOUT QUADRATIC HAMILTONIANS

For the time-dependent Hamiltonian in Eq. (1), it is easy to calculate the ''equations of motion'' using Eq. (3):

$$\dot{\hat{x}}=a\hat{p}+b\hat{x}+f,\quad -\dot{\hat{p}}=b\hat{p}+c\hat{x}+g. \tag{6}$$

These have exactly the same form as the corresponding classical equations (i.e., Hamiltonian's equations). It follows from Eq. (4) that the expectation values of position and momentum exactly follow a classical trajectory. This is essentially Ehrenfest's result for this system.

For any wave packet define $\hat{X}:=\hat{x}-\langle\hat{x}\rangle$, $\hat{P}:=\hat{p}-\langle\hat{p}\rangle$. Then, from Eq. (6),

$$\dot{\hat{X}}=a\hat{P}+b\hat{X},\quad -\dot{\hat{P}}=b\hat{P}+c\hat{X}, \tag{7}$$

i.e., $\hat{X},\hat{P}$ satisfy the undriven equations of motion. [The terms involving f or g will be referred to as ''driving'' terms.] Since these equations for $\hat{X}$ and $\hat{P}$ do not depend on $\hat{x}$ or $\hat{p}$, the motion of the centroid (defined by $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$) is separate from that of any moment relative to the centroid, i.e., the expectation value of any operator built from $\hat{X}$ and $\hat{P}$. For example, it is shown in the Appendix that the spreads in position and momentum ($\Delta_x:=\langle\hat{X}^2\rangle^{1/2}$ and $\Delta_p:=\langle\hat{P}^2\rangle^{1/2}$) evolve independently of the centroid and are completely unaffected by f or g. This is an important simplifying feature of the evolution with quadratic Hamiltonians; it has been noted[9] for a homogeneous time-varying force and another example will be considered in Sec. IX D. Furthermore, the evolution of the spreads can be expressed in terms of solutions of the classical equations of motion. It is shown in the Appendix that the spreads exactly follow those for a set of identical classical particles subject to the corresponding classical Hamiltonian. Since the centroid and spreads of a wave packet follow exactly those of a set of classical particles and can be calculated from the classical equations of motion, it is not surprising that the complete evolution of the wave packet can also be calculated from the classical equations of motion.

It has long been known that there is a way of mapping any wave function into a distribution in phase space (sometimes negative!) that evolves classically in the case of a quadratic Hamiltonian. This is provided by the Wigner distribution

$$W(x,p,t):=\frac{1}{h}\int e^{-ipy/h}\psi\left(x+\frac{1}{2}y\right)\psi^*\left(x-\frac{1}{2}y\right)dy. \tag{8}$$

It has been shown[10] that this satisfies the classical Liouville equation if the Hamiltonian is quadratic. This means that the distribution evolves as if each point in phase space follows the trajectory of a classical particle.[11] This connection will not be pursued here; instead we will find the evolution of wave functions by introducing an invariant operator.

IV. INVARIANT OPERATORS

An operator is said to be invariant if its total time derivative is zero; in Eq. (3) the intrinsic time dependence of the operator cancels that from the commutator. Invariant operators corresponds to constants of the motion in the sense that (i) the expectation value with respect to any state is constant, which follows from Eq. (4), and (ii) any eigenstate of an invariant operator will remain an eigenstate (with unchanging eigenvalue). To see this observe that

$$\left(\hat{H}-i\hbar\frac{\partial}{\partial t}\right)\hat{A}\psi=\left(\hat{H}\hat{A}-i\hbar\frac{\partial\hat{A}}{\partial t}-\hat{A}\hat{H}\right)\psi=-i\hbar\dot{\hat{A}}\psi. \tag{9}$$

So, if $\hat{A}$ is invariant and ψ satisfies Schrödinger's equation then so does $\hat{A}\psi$. Therefore, if $\hat{A}\psi-\alpha\psi=0$ at some time, then it must remain zero. Similarly, if a relation of the form $\hat{A}\psi=\phi$ holds at some time, then it will hold at all times (assuming ψ, ϕ obey Schrödinger's equation).

V. INVARIANT OPERATORS FOR QUADRATIC HAMILTONIANS

It will now be shown that it is possible to construct an invariant of the form

$$\hbar\hat{a}=\xi\hat{p}-\pi\hat{x}+\hbar\sigma, \tag{10}$$

where ξ, π, σ, are functions of the time. Using the equations of motion, Eq. (6), it follows that

$$\hbar\dot{\hat{a}}=(\dot{\xi}-b\xi-a\pi)\hat{p}-(\dot{\pi}+c\xi+b\pi)\hat{x}+(\hbar\dot{\sigma}-g\xi-f\pi)$$

and therefore $\hat{a}$ will be invariant if

$$\begin{aligned} \dot{\xi} &= a\pi + b\xi, \\ -\dot{\pi} &= b\pi + c\xi, \\ \hbar\dot{\sigma} &= f\pi + g\xi. \end{aligned} \tag{11}$$

[For the common case where $b=0$, one can replace π by $m\dot{\xi}$.] That is, ξ and π must satisfy the equations of motion for the classical undriven system (i.e., homogeneous, with $f=g=0$) and then

$$\hbar\sigma = \int_0^t (f\pi + g\xi)\,dt. \tag{12}$$

Any lower limit could be used in this integration; this choice makes $\sigma=0$ at $t=0$. Thus from any two solutions of the classical undriven system, one can build an invariant of the quantum system, including the driving.

Now $\hbar[\hat{a},\hat{a}^\dagger] = i(\xi\pi^* - \xi^*\pi)$. This must be constant (because $\hat{a}$ and $\hat{a}^\dagger$ are invariant) and real. Therefore the required classical solutions can be taken to be complex and scaled to make

$$i(\xi\pi^* - \xi^*\pi) = \hbar,$$

i.e.,

$$\mathrm{Im}(\xi^*\pi) = \tfrac{1}{2}\hbar, \tag{13}$$

and then

$$[\hat{a},\hat{a}^\dagger] = 1. \tag{14}$$

VI. EIGENFUNCTIONS OF INVARIANT OPERATORS

Let ψ_α^0 be the eigenstate of $\hat{a}$ with eigenvalue α, so that

$$\hat{a}\psi_\alpha^0 = \alpha\psi_\alpha^0. \tag{15}$$

It is convenient to define $\hat{a}_\alpha := \hat{a} - \alpha$. Then $\hat{a}_\alpha$ is invariant, $\hat{a}_\alpha\psi_\alpha^0 = 0$, and

$$[\hat{a}_\alpha,\hat{a}_\alpha^\dagger] = 1. \tag{16}$$

As in the case of the harmonic oscillator, one can now generate the infinite set of orthonormal eigenstates of $\hat{a}_\alpha^\dagger\hat{a}_\alpha$ (with eigenvalue n):

$$\psi_\alpha^n = \frac{1}{\sqrt{n!}}(\hat{a}_\alpha^\dagger)^n\psi_\alpha^0 \quad \text{with} \quad n = 1,2,3,\ldots. \tag{17}$$

The states ψ_α^n remain eigenstates of $\hat{a}_\alpha^\dagger\hat{a}_\alpha$, and relations between them of the form

$$\psi_\alpha^{n+1} = \frac{1}{\sqrt{n}}\,\hat{a}_\alpha^\dagger\psi_\alpha^n \tag{18}$$

remain true as the states evolve, because $\hat{a}_\alpha^\dagger$ is invariant, as in Eq. (9).

This is the heart of the matter; we have constructed an infinite string of states that follow the motion (with continuously changing parameters ξ, π) but retain the algebraic relations that will be seen to preserve the simple form of their wave functions.

A. Expectation values

It will emerge that these eigenfunctions ψ_α^n can be completely characterized by their expectation values of $\hat{x}$ and $\hat{p}$, and the spreads Δ_x and Δ_p. These are easily determined, as follows.

First, note that

$$\langle\hat{a}\rangle = \alpha, \quad \langle\hat{a}^\dagger\rangle = \alpha^* \quad \text{for all } n, \tag{19}$$

because $\langle\hat{a}\rangle = \langle\hat{a}_\alpha\rangle + \alpha$ and $\langle\hat{a}_\alpha\rangle = 0$ since $\hat{a}_\alpha$ lowers the eigenstate to an orthogonal one.

Equation (10) and its adjoint can be solved for $\hat{x}$ and $\hat{p}$, using Eq. (13):

$$\begin{aligned} \hat{x} &= i(\xi^*\hat{a} - \xi\hat{a}^\dagger) - i(\xi^*\sigma - \xi\sigma^*), \\ \hat{p} &= i(\pi^*\hat{a} - \pi\hat{a}^\dagger) - i(\pi^*\sigma - \pi\sigma^*), \end{aligned} \tag{20}$$

and therefore

$$\begin{aligned} \hat{X} &:= \hat{x} - \langle\hat{x}\rangle = i(\xi^*\hat{a}_\alpha - \xi\hat{a}_\alpha^\dagger), \\ \hat{P} &:= \hat{p} - \langle\hat{p}\rangle = i(\pi^*\hat{a}_\alpha - \pi\hat{a}_\alpha^\dagger). \end{aligned} \tag{21}$$

Now it is easy to calculate the second-order moments, using $\langle\hat{a}_\alpha^\dagger\hat{a}_\alpha\rangle = n$,

$$\begin{aligned} \Delta_x^2 &:= \langle\hat{X}^2\rangle = \xi^*\xi(2n+1), \\ \Delta_{xp} &:= \langle\tfrac{1}{2}(\hat{P}\hat{X} + \hat{X}\hat{P})\rangle = \zeta(2n+1), \\ \Delta_p^2 &:= \langle\hat{P}^2\rangle = \pi^*\pi(2n+1), \end{aligned} \tag{22}$$

where $\zeta := \mathrm{Re}(\xi^*\pi)$. From this definition of ζ and Eq. (13) it follows that

$$\xi^*\pi = \zeta + \tfrac{1}{2}i\hbar. \tag{23}$$

Hence, for these eigenstates, the three moments are related:

$$\Delta_x^2\Delta_p^2 - \Delta_{xp}^2 = \tfrac{1}{4}\hbar^2(2n+1). \tag{24}$$

In the Appendix, this relation is compared with the corresponding one for an arbitrary wave packet. Equation (22) shows that the classical solution ξ, π determines the spread of the wave packets, and then Eq. (20) shows that the eigenvalue α determines $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$.

B. Wave functions

Equation (10), minus its expectation value, becomes

$$\hbar\hat{a}_\alpha = \xi(\hat{p} - \overline{p}) - \pi(\hat{x} - \overline{x}), \tag{25}$$

where $\overline{p} := \langle\hat{p}\rangle$, $\overline{x} := \langle\hat{x}\rangle$. In Schrödinger's representation, where $\hat{p} = -i\hbar\,\partial/\partial x$, the solution of $\hat{a}_\alpha\psi_\alpha^0 = 0$ is therefore, apart from normalization,

$$\psi_\alpha^0 = \exp\left[\frac{i\pi}{2\hbar\xi}\left(x - \overline{x} + \frac{\xi}{\pi}\,\overline{p}\right)^2\right]. \tag{26}$$

This is more easily understood if it is expressed as a real Gaussian multiplied by a phase factor (that varies with x). The exponent in Eq. (26) is

$$\begin{aligned} &\frac{i}{2\hbar}\left[\frac{\pi}{\xi}(x-\overline{x})^2 + 2\overline{p}(x-\overline{x}) + \frac{\xi}{\pi}\,\overline{p}^2\right] \\ &\quad = i\theta - \left[\left(\frac{x-\overline{x}}{2|\xi|}\right)^2 - \left(\frac{\overline{p}}{2|\pi|}\right)^2\right], \end{aligned}$$

where

$$\theta := \frac{1}{2\hbar}\left[\zeta\left(\frac{x-\overline{x}}{|\xi|}\right)^2 + 2\overline{p}(x-\overline{x}) + \zeta\left(\frac{\overline{p}}{|\pi|}\right)^2\right]. \tag{27}$$

Here we have used, from Eq. (23),

$$\begin{aligned}\pi/\xi &= \xi^*\pi/|\xi|^2 = (\zeta = \tfrac{1}{2}i\hbar)/|\xi|^2,\\ \xi/\pi &= \xi\pi^*/|\pi|^2 = (\zeta - \tfrac{1}{2}i\hbar)/|\pi|^2.\end{aligned} \tag{28}$$

Therefore,

$$\psi_\alpha^0 = e^{i\theta}\exp[-\{\tfrac{1}{2}(x-\overline{x})/|\xi|\}^2]\exp[\{\tfrac{1}{2}\overline{p}/|\pi|\}^2]. \tag{29}$$

The last term will be absorbed into the normalization of ψ_α^0.

To deal with the states with $n>0$, we need[12] the effect of interchanging $\hat{a}_\alpha$ and $e^{i\theta}$.

From $[\hat{a}, e^{i\theta(x)}] = \hbar^{-1}\xi[\hat{p}, e^{i\theta(x)}] = \xi\theta'$ it follows that, for any wave function ψ,

$$\begin{aligned}\hat{a}_\alpha e^{i\theta}\psi &= e^{i\theta}(\hat{a}_\alpha + \xi\theta')\psi\\ &= e^{i\theta}\frac{\xi}{\hbar}\left\{\left[\hat{p} - \overline{p} - \frac{\pi}{\xi}(x-\overline{x})\right] + \left[\zeta\frac{(x-\overline{x})}{|\xi|^2} + \overline{p}\right]\right\}\psi\\ &= e^{i\theta}\frac{\xi}{\hbar}\left\{\hat{p} - \frac{i\hbar}{2|\xi|^2}(x-\overline{x})\right\}\psi,\end{aligned}$$

where we have again used Eq. (28). Thus

$$\hat{a}_\alpha e^{i\theta}\psi = e^{i(\theta+\beta)}\hat{\mathfrak{a}}\psi, \tag{30}$$

where

$$\hat{\mathfrak{a}} := \frac{|\xi|}{\hbar}\hat{p} - \frac{i}{2|\xi|}(x-\overline{x}), \tag{31}$$

and β is the phase of ξ, so that

$$e^{i\beta} = \xi/|\xi|. \tag{32}$$

It is easily verified that $[\hat{\mathfrak{a}}, \hat{\mathfrak{a}}^\dagger] = 1$ and it is possible to construct a basis $\phi_{|\xi|}^n(x-\overline{x})$ of real eigenstates of $\hat{\mathfrak{a}}^\dagger\hat{\mathfrak{a}}$ such that $\hat{\mathfrak{a}}\phi_{|\xi|}^0 = 0$ and $\phi_{|\xi|}^{n+1} := n^{-1/2}\hat{\mathfrak{a}}\phi_{|\xi|}^n$. These, of course, are just the ordinary oscillator eigenstates, centered on $\overline{x}$, with scale set by $|\xi|$. They can be expressed in terms of the Hermite polynomials:[13]

$$\begin{aligned}\phi_{|\xi|}^n(y) &= (2\pi)^{-1/4}|\xi|^{-1/2}2^{-n/2}(n!)^{-1/2}\\ &\quad\times\exp(-\tfrac{1}{4}|\xi|^{-2}y^2)H_n(2^{-1/2}|\xi|^{-1}y).\end{aligned} \tag{33}$$

Now the complex eigenstates ψ_α^n of $\hat{a}_\alpha^\dagger\hat{a}_\alpha$ can be expressed in terms of the real $\phi_{|\xi|}^n$ as

$$\psi_\alpha^n := e^{i(\theta+n\beta)}\phi_{|\xi|}^n(x-\overline{x}), \tag{34}$$

because then Eq. (30) shows that Eqs. (15) and (18) are satisfied.

[Proof: $\hat{a}_\alpha\psi_\alpha^0 = \hat{a}_\alpha e^{i\theta}\phi_{|\xi|}^0 = e^{i(\theta+\beta)}\hat{\mathfrak{a}}\phi_{|\xi|}^0 = 0$ and $\psi_\alpha^{n+1} = e^{i[\theta+(n+1)\beta]}\phi_{|\xi|}^{n+1} = n^{-1/2}e^{i[\theta+(n+1)\beta]}\hat{\mathfrak{a}}\,\phi_{|\xi|}^n = n^{-1/2}\hat{a}_\alpha \times e^{i(\theta+n\beta)}\phi_{|\xi|}^n = n^{-1/2}\hat{a}_\alpha\psi_\alpha^n$.]

Note that ψ_α^n retains the form given in Eq. (34) for all time, but ξ and π change with time (on a classical trajectory) and therefore so do θ, β, and ζ. It is remarkable that any Gaussian or Hermite–Gaussian wave packet will retain its form even with arbitrary time variation of the forces (or the mass) as long as the dependence of the Hamiltonian on x and p remains quadratic.

VII. THE EVOLUTION OF AN ARBITRARY WAVE FUNCTION

For any complex solution ξ, π (of the undriven system) and any eigenvalue α, the set ψ_α^n for $n=1,2,3,...$ is complete. Therefore the time-evolution $\Psi(x,t)$ of any wave function $\Psi(x,0)$, given at time $t=0$, can be obtained by expanding it in terms of the $\psi_\alpha^n(x,0)$. Thus, if

$$\Psi(x,0) = \sum_n c_n\psi_\alpha^n(x,0) \tag{35}$$

then

$$\Psi(x,t) = \sum_n c_n\psi_\alpha^n(x,t). \tag{36}$$

For some purposes it might be possible to take just a few terms of this expansion to give a wave packet of desired form by a suitable choice of the c_n, and then Eq. (36) can be used directly. If the exact evolution of an arbitrary initial wave function $\Psi(x,0)$ is required then the orthonormality of the ψ_α^n can be used to find the c_n:

$$c_n = \int_{-\infty}^{\infty}\psi_\alpha^n{}^*(x,0)\Psi(x,0)dx. \tag{37}$$

Although the basis is complete for any choice of ξ_0, π_0, and α, one would naturally choose these to match the spreads and means of the wave packet, particularly if numerical calculations were to be undertaken.

The propagator. Inserting (37) into Eq. (36) gives

$$\Psi(x,t) = \int_{-\infty}^{\infty}K(x,x',t)\Psi(x',0)dx', \tag{38}$$

where

$$\begin{aligned}K(x,x',t) &= \sum_n \psi_\alpha^n(x,t)\psi_\alpha^n{}^*(x',0)\\ &= e^{i\Delta\theta}\sum_n e^{in\Delta\beta}\phi_{|\xi|}^n(x-\overline{x})\,\phi_{|\xi'|}^n(x'-\overline{x}'),\end{aligned} \tag{39}$$

where $\Delta\theta := \theta(x,t) - \theta(x',0)$ and $\Delta\beta := \beta(t) - \beta(0)$. Writing $y := (x-\overline{x})/(\sqrt{2}|\xi|)$ and inserting Eq. (33) gives

$$\begin{aligned}K(x,x',t) &= \frac{e^{i\Delta\beta}}{\sqrt{2\pi|\xi\xi'|}}\exp-[\tfrac{1}{2}(y^2+y'^2)]\\ &\quad\times\sum_n\frac{e^{in\Delta\beta}}{2^n n!}H_n(y)H_n(y').\end{aligned} \tag{40}$$

This sum can be carried out exactly using Mehler's formula:[14]

$$\begin{aligned}&\sum_n\frac{z^n}{2^n n!}H_n(y)H_n(y')\\ &= \frac{1}{\sqrt{1-z^2}}\exp\left\{\frac{2zyy' - z^2(y^2+y'^2)}{1-z^2}\right\},\end{aligned} \tag{41}$$

which leads to

$$K(x,x',t)=\frac{1}{\sqrt{-4\pi i|\xi\xi'|\sin\Delta\beta}}\exp\left\{i\left[\Delta\theta-\frac{1}{2}\Delta\beta+\frac{2yy'-(y^2+y'^2)\cos\Delta\beta}{2\sin\Delta\beta}\right]\right\}. \tag{42}$$

This is not the most useful form for the propagator, because there are cancellations between $\Delta\theta$ and the last term. A more direct method will be given elsewhere.

VIII. DETERMINING ξ, π

To deal with specific examples, it helps to express the required classical solution ξ, π (of the undriven system) in terms of a standard basis of real solutions. In the present one-dimensional case, two real solutions are needed. In this section, it will be assumed that there is no cross term in the Hamiltonian ($b=0$). Then the undriven equations of motion are

$$p=m\dot{x}, \quad \dot{p}=-cx \tag{43}$$

(m and c may vary with time). We can take the real basis of solutions of this to be $x=u(t)$ with $u(0)=1$, $\dot{u}(0)=0$, and $x=\nu(t)$ with $\nu(0)=0$, $m_0\dot{\nu}(0)=1$. The complex solution ξ must be a linear combination of these and, since a constant phase factor can be removed, we can take

$$\xi=\Delta u+e^{i\varphi}\Box\nu, \quad \pi=m(\Delta\dot{u}+e^{i\varphi}\Box\dot{\nu}), \tag{44}$$

where Δ, $\Box$, φ are constants. From Eq. (22), Δ is the initial value of Δ_x for any $n=0$ state, and $\Box$ is the initial value of Δ_p. To satisfy the normalization condition Eq. (13), we require

$$\Delta\Box\ \sin\varphi=\tfrac{1}{2}\hbar. \tag{45}$$

Thus there are only two parameters to be chosen to determine the solution and these could be Δ and $\Box$, the initial spreads in position and momentum. The initial value of $\zeta:=\mathrm{Re}(\xi^*\pi)$ is

$$\zeta_0=\Delta\Box\ \cos\varphi. \tag{46}$$

In terms of this,

$$\xi=\Delta u+\Delta^{-1}[\zeta_0+\tfrac{1}{2}i\hbar]\nu, \tag{47}$$

and

$$\Delta^2\Box^2=\zeta_0^2+\tfrac{1}{4}\hbar^2, \tag{48}$$

as in Eq. (24).

Expectation values of position and momentum follow the classical motion and therefore

$$\overline{x}\equiv\langle\mathbf{x}\rangle=\overline{x_0}u+\overline{p_0}\nu,$$
$$\overline{p}\equiv\langle\mathbf{p}\rangle=m(\overline{x_0}\dot{u}+\overline{p_0}\dot{\nu}). \tag{49}$$

The second-order moments for any $n=0$ state, given in Eq. (22), now work out to be

$$\xi^*\xi=\Delta^2u^2+2\zeta_0u\nu+\Box^2\nu^2,$$
$$\zeta=m[\Delta^2u\dot{u}+\zeta_0(u\dot{\nu}+\dot{u}\nu)+\Box^2\nu\dot{\nu}], \tag{50}$$
$$\pi^*\pi=m^2[\Delta^2\dot{u}^2+2\zeta_0\dot{u}\dot{\nu}+\Box^2\dot{\nu}^2],$$

agreeing with Eq. (A4) for an arbitrary wave packet.

The generic form of the eigenfunctions is more easily found if the origin of time is taken to be when $\zeta=0$, so that $\zeta_0=0$. Then, by Eq. (48), $\Delta\Box=\frac{1}{2}\hbar$ and therefore any $n=0$ state is a minimum-uncertainty state at that time. Also it follows from Eqs. (45) and (46) that $\cos\phi=0$ and $\sin\phi=1$ and therefore $\xi=\Delta u+i\Box\nu$, where $\Box=\frac{1}{2}\hbar\Delta^{-1}$. (In the cases examined in this paper, no loss of generality is caused by this assumption that there is a finite time for which $\zeta=0$, which implies that there is some time when the $n=0$ state has the minimum possible uncertainty product. It is unknown to me whether this is true for any quadratic Hamiltonian.)

IX. EXAMPLES OF UNDRIVEN SYSTEMS (WITH $b=0$)

The steps to be taken to find the set of wave packets ψ_α^n and their evolution are as follows.

(1) Solve the classical equations of motion $(d/dt)(m\dot{x})=-cx$ for u, ν. (If this cannot be done analytically, then a computed solution will do.)
(2) Choose the initial spread Δ. (It is being assumed that the initial time will be such that $\zeta_0=0$.) This determines ξ,π with $\xi=\Delta u+i\Box\nu$, $\pi=m\dot{\xi}$, and $\Box=\frac{1}{2}\hbar\Delta^{-1}$.
(3) Choose the initial means $\overline{x_0},\overline{p_0}$. Then the invariant eigenvalue is, from Eq. (10), $\hbar\alpha=\Delta\overline{p_0}-i\Box\overline{x_0}$.
(4) Then the infinite set of wave packets is given by Eqs. (34) and (33).

A. Free particle ($\ddot{x}=0$, $u=1$, $\nu=t/m$)

The motion of the centroid is very simple: $\overline{p}=\overline{p_0}$, $\overline{x}=\overline{x_0}+m^{-1}\overline{p_0}t$. Also

$$\xi=\Delta+im^{-1}\Box t, \quad \pi=i\Box, \quad \zeta=m^{-1}\Box^2t, \tag{51}$$

and therefore

$$|\xi|^2=\Delta^2+m^{-2}\Box^2t^2. \tag{52}$$

The spread in momentum does not change with time. Spatially, the packet narrows and then spreads. At its minimum spread, it has the minimum uncertainty product.

The Gaussian solution of the free Schrödinger equation is discussed in many texts.[15] The Hermite–Gaussians have had little (if any?) attention in quantum mechanics but they are well known in the wave optics of axisymmetric optical systems, where the paraxial wave equation takes the form of a one-dimensional free Schrödinger equation (with time replaced by distance along the axis).[16]

B. Damped free particle

As an example of a time-dependent undriven system, consider the Hamiltonian $\hat{H}=e^{-\gamma t}\hat{p}^2/2m$. This is the Caldirola–Kanai Hamiltonian for the damped motion of a free particle.[17] The classical equations of motion are $p=e^{\gamma t}m\dot{x}$ and $\dot{p}=0$, which lead to $\ddot{x}+\gamma\dot{x}=0$. Thus γ gives the strength of the damping force. The basis of solutions of this is $u=1$ and $\nu=(1-e^{-\gamma t})/m\gamma$. Hence $\overline{p}=\overline{p_0}$, $\overline{x}=\overline{x_0}+m^{-1}\overline{p_0}\tau$, where $\tau:=(1-e^{-\gamma t})/\gamma$. Also

$$\xi=\Delta+im^{-1}\Box\tau, \quad \pi=i\Box e^{-\gamma t}, \quad \zeta=m^{-1}\Box^2e^{-\gamma t}\tau. \tag{53}$$

For small γ these quantities revert to those for the undamped case. Note that the spread of the packet, measured by $|\xi|$, tends to a constant value at large times. The evolution of a

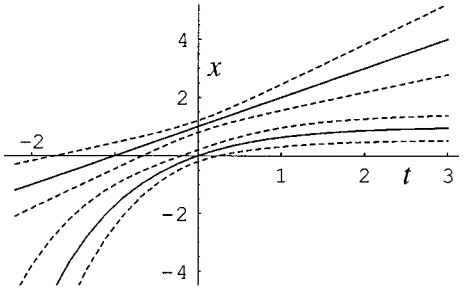

Fig. 1. Evolution of a Gaussian wave function for a free particle (the top three curves) arranged to have $\langle\hat{x}\rangle$ pass through $x=1$ at $t=0$ and to have its minimum spread there. Also (the bottom three curves) the similar evolution for a damped free particle arranged to pass through $x=0$ at $t=0$. In both cases the dashed curves give the trajectory of the points where $x=\langle\hat{x}\rangle \pm 2|\xi|$, i.e., the points where the Gaussian falls off to $1/e$ of its central value. (The parameters are $m=p=\gamma=1$, $\Delta=0.1$, $\square=0.2$.)

typical wave packet is compared with that for the undamped case in Fig. 1. A model of the Brownian motion of a quantum particle results from adding a stochastic driving force;[17] this also comes within the scope of the present method.

C. Harmonic oscillator [m and ω constant: $\ddot{x}=-\omega^2 x$, $u=\cos\omega t$, $\nu=(\omega m)^{-1}\sin\omega t$]

Write $L:=\sqrt{2m\omega/\hbar}$ (with the dimensions of length) and $s:=\Delta/L$ (sometimes called the squeezing factor). Then

$$\begin{aligned}\xi&=L(s\cos\omega t+is^{-1}\sin\omega t),\\ \pi&=m\omega L(-s\sin\omega t+is^{-1}\cos\omega t),\\ \zeta&=\tfrac{1}{4}\hbar(s^{-2}-s^2)\sin 2\omega t.\end{aligned}\tag{54}$$

So the spreads oscillate with angular period 2ω. Unless $\alpha=0$ these states are (or will be) spatially displaced from the centre of the oscillator; they correspond to what are called *displaced number states* in quantum optics.[4] If $s=1$ then $\zeta=0$ for all time and $\xi=Le^{i\omega t}$ so $|\xi|$ and $|\pi|$ do not change with time; these are called *coherent states*. If $s\neq 1$ they are called *squeezed states*.

The displaced oscillator ground state was discovered by Schrödinger[18] in 1926, the squeezed equivalent was found by Kennard[19] in 1927, and displaced number states were discovered by Senitzky[20] in 1954.

D. Parabolic hill [$\ddot{x}=\lambda^2 x$, $u=\cosh\lambda t$, $\nu=(m\lambda)^{-1}\sinh\lambda t$]

$$\begin{aligned}\xi&=\Delta\cosh\lambda t+i(m\lambda)^{-1}\sinh\lambda t,\\ \zeta&=\tfrac{1}{2}m\lambda[\Delta^2+(m\lambda)^{-2}\square^2]\sinh 2\lambda t.\end{aligned}\tag{55}$$

The width of the packet narrows and then spreads, as does the free particle; but here the rate of spreading is ultimately exponential with time instead of linear. This is an interesting case in which to contemplate the separation of the motion of the centroid from that of the moments (relative to the centroid). The spreads evolve independently of whether the centroid goes over the hill or retreats before the top. In the case of two classical particles starting together with different velocities, their distance apart goes as $\sinh\lambda t$ whether they both go over the hill or one goes over and the other falls back! Also, in the quantum case the wave packet remains Gaussian[21] (or Gauss–Hermite) in either case!

X. DRIVEN SYSTEMS

All higher moments, i.e., averages over products of deviations from the mean, are the same as for the corresponding undriven system. Only the effects of the driving on $\overline{x}$ and $\overline{p}$ need be considered and this is essentially an exercise in classical mechanics. From Eq. (20),

$$\overline{x}=\bar{\bar{x}}+2\,\mathrm{Im}(\xi^*\sigma),\quad \overline{p}=\bar{\bar{p}}+2\,\mathrm{Im}(\pi^*\sigma),\tag{56}$$

where $\bar{\bar{x}},\bar{\bar{p}}$ are the mean position and momentum for the undriven system. Using Eq. (12),

$$\begin{aligned}\mathrm{Im}(\xi^*\sigma)&=\hbar^{-1}\int_0^t\{\mathrm{Im}(\xi^*(t)\xi(t'))g(t')\\ &\quad+\mathrm{Im}(\xi^*(t)\pi(t'))f(t')\}dt',\\ \mathrm{Im}(\pi^*\sigma)&=\hbar^{-1}\int_0^t\{\mathrm{Im}(\pi^*(t)\xi(t'))g(t')\\ &\quad+\mathrm{Im}(\pi^*(t)\pi(t'))f(t')\}dt'.\end{aligned}\tag{57}$$

It is convenient to write this as

$$\begin{aligned}\mathrm{Im}(\xi^*\sigma)&=\frac{1}{2}\int_0^t\{A(t,t')g(t')+B(t,t')f(t')\}dt',\\ \mathrm{Im}(\pi^*\sigma)&=\frac{1}{2}\int_0^t\{-B(t',t)g(t')+C(t,t')f(t')\}dt',\end{aligned}\tag{58}$$

where

$$\begin{aligned}A(t,t')&:=2\hbar^{-1}\,\mathrm{Im}(\xi^*(t)\xi(t')),\\ B(t,t')&:=2\hbar^{-1}\,\mathrm{Im}(\xi^*(t)\pi(t')),\\ C(t,t')&:=2\hbar^{-1}\,\mathrm{Im}(\pi^*(t)\pi(t')).\end{aligned}\tag{59}$$

In terms of the basis u, ν of classical solutions (for $b=0$)

$$\begin{aligned}A(t,t')&=u(t)\nu(t')-\nu(t)u(t'),\\ B(t,t')&=m[u(t)\dot{\nu}(t')-\nu(t)\dot{u}(t')],\\ C(t,t')&=m^2[\dot{u}(t)\dot{\nu}(t')-\dot{\nu}(t)\dot{u}(t')]\end{aligned}\tag{60}$$

and, by Eq. (49),

$$\bar{\bar{x}}=\overline{x_0}u+\overline{p_0}\nu,\quad \bar{\bar{p}}=m(\overline{x_0}\dot{u}+\overline{p_0}\dot{\nu}).\tag{61}$$

XI. EXAMPLES OF DRIVEN SYSTEMS

A. Motion under gravity

With our definition of driving, this is a free particle with a constant driving term g. Thus u and ν are as for the free particle and then

$$A(t,t')=(t'-t)/m,\quad B(t,t')=1,\quad C(t,t')=0.\tag{62}$$

Evaluating the integrals in Eq. (58) and adding to Eq. (61) gives

$$\overline{x}=\overline{x_0}+m^{-1}\overline{p_0}t-\frac{1}{2m}gt^2,\quad \overline{p}=\overline{p_0}-gt,\tag{63}$$

as expected.

B. Time-varying, spatially homogeneous field (Ref. 9)

This case is the same as in Sec. X A except that g now varies with time,

$$\overline{x}=\overline{x_0}+m^{-1}\overline{p_0}t-m^{-1}\int_0^t(t-t')g(t')dt',$$
$$\overline{p}=\overline{p_0}-\int_0^t g(t')dt'. \tag{64}$$

C. Driven oscillator (Ref. 5)

Consider the driving to be through a term $g(t)x$ in the Hamiltonian. The undriven case was dealt with in Sec. IX C. Hence,

$$A(t,t')=(\omega m)^{-1}\sin[\omega(t-t')],$$
$$B(t,t')=\cos[\omega(t-t')], \tag{65}$$
$$C(t,t')=\omega m\sin[\omega(t-t')],$$

and therefore

$$\overline{x}=\overline{x_0}\cos\omega t+(m\omega)^{-1}\overline{p_0}\sin\omega t+(m\omega)^{-1}\int_0^t\sin[\omega(t'-t)]g(t')dt',$$
$$\overline{p}=-m\omega\overline{x_0}\sin\omega t+\overline{p_0}\cos\omega t-\int_0^t\cos[\omega(t'-t)]g(t')dt'. \tag{66}$$

XII. CONCLUSION

It has been shown that, for any quadratic Hamiltonian, one can form a time-dependent invariant operator $\hat{a}$, using trajectories of the corresponding classical system. This enables the construction of wave packets (with the form of oscillator eigenstates) that follow the classical motion (as do all normalisable wave packets). The evolution of any wave function can also be calculated through the explicit propagator. Thus, every detail of the evolution of a quantum quadratic system can be calculated from the trajectories of the corresponding classical system. The initial values, however, are subject to constraints (such as the uncertainty relations) that are not present for the classical system.

The method used is applicable for arbitrary time dependence in the Hamiltonian and it makes little difference to the development of the theory whether such time dependence is present or not; $\hat{a}$ will vary with time in either case. Even in the case of a time-independent Hamiltonian this method has advantages over the usual method of expanding in eigenstates of the Hamiltonian in that the states used here are wave packets following the classical motion. Thus in the case of a free particle the energy eigenstates are plane waves, whereas in the present method the Gaussian packet and the Gauss–Hermite packets emerge. In the case of the harmonic oscillator, the displaced oscillator ground state, the squeezed states, and the displaced number states emerge.

APPENDIX: MOMENTS OF ARBITRARY WAVE PACKETS

It is shown here that the second-order moments of an arbitrary wave packet have some simple properties for quadratic Hamiltonians. From Eqs. (5) and (7),

$$\frac{d}{dt}(\hat{X}^2)=a(\hat{P}\hat{X}+\hat{X}\hat{P})+2b\hat{X}^2,$$
$$\frac{d}{dt}(\hat{P}\hat{X}+\hat{X}\hat{P})=2a\hat{P}^2-2c\hat{X}^2, \tag{A1}$$
$$\frac{d}{dt}(\hat{P}^2)=-2b\hat{P}^2-c(\hat{P}\hat{X}+\hat{X}\hat{P}).$$

Thus, defining the second-order moments Δ_x, Δ_p, Δ_{xp} as in Eq. (22),

$$\frac{d}{dt}\Delta_x^2=2a\Delta_{xp}+2b\Delta_x^2,$$
$$\frac{d}{dt}\Delta_{xp}=a\Delta_p^2-c\Delta_x^2, \tag{A2}$$
$$\frac{d}{dt}\Delta_p^2=-2b\Delta_p^2-2c\Delta_{xp}.$$

The product of any two solutions x_1,p_1 and x_2,p_2 of the classical undriven equations, $\dot{x}=ap+bx$, $-\dot{p}=bp+cx$, will satisfy Eq. (A2); this is easily seen because the algebra is the same as for Eq. (A1). If these two classical solutions are independent, then x_1^2,x_1x_2,x_2^2 will provide a basis for Δ_x^2 and so on, so that we can write

$$\Delta_x^2=Ax_1^2+2Bx_1x_2+Cx_2^2,$$
$$\Delta_{xp}=Ax_1p_1+B(x_1p_2+x_2p_1)+Cx_2p_2, \tag{A3}$$
$$\Delta_p^2=Ap_1^2+2Bp_1p_2+Cp_2^2.$$

If the solutions x_1,p_1 and x_2,p_2 are chosen so that initially $x_1(0)=1$, $p_1(0)=0$ and $x_2(0)=0$, $p_2(0)=1$, then putting A, B, C equal to the initial values of Δ_x^2, Δ_{xp}, Δ_p^2 will satisfy the initial conditions of Eq. (A3). That is,

$$\Delta_x^2=\Delta_x^{0^2}x_1^2+2\Delta_{xp}^0x_1x_2+\Delta_p^{0^2}x_2^2,$$
$$\Delta_{xp}=\Delta_x^{0^2}x_1p_1+\Delta_{xp}^0(x_1p_2+x_2p_1)+\Delta_p^{0^2}x_2p_2, \tag{A4}$$
$$\Delta_p^2=\Delta_x^{0^2}p_1^2+2\Delta_{xp}^0p_1p_2+\Delta_p^{0^2}p_2^2.$$

Thus the evolution of the second-order moments of an arbitrary wave packet is simply expressed in terms of classical trajectories.

The initial values of these three second-order moments are initially independent, but they do not evolve independently; it is easily derived from Eq. (A2) that $\Delta_x^2\Delta_p^2-\Delta_{xp}^2$ is constant. Furthermore this quantity satisfies the inequality

$$\Delta_x^2\Delta_p^2-\Delta_{xp}^2\geqslant\tfrac{1}{4}\hbar^2. \tag{A5}$$

This can be derived from a form of Schwarz's inequality,

$$4\langle\hat{P}^2\rangle\langle\hat{X}^2\rangle\geqslant\langle\hat{P}\hat{X}+\hat{X}\hat{P}\rangle^2|\langle\hat{P}\hat{X}-\hat{X}\hat{P}\rangle|^2. \tag{A6}$$

It is interesting that Schrödinger noted[22] in 1930 that this inequality is stronger than Heisenberg's uncertainty inequality. Equation (24) shows that the $n=0$ states saturate the inequality in Eq. (A5) in the sense that equality holds at all times.[23]

A set of N identical classical particles moving under this Hamiltonian will have the same evolution equations for their moments, defined by $\overline{x}:=N^{-1}\Sigma_i x^i$, $\Delta_x^2:=N^{-1}\Sigma_i(x^i-\overline{x})^2$,

etc. In this case $\Delta_x^2\Delta_p^2-\Delta_{xp}^2$ is constant, but must be non-negative (rather than not less than $\frac{1}{4}\hbar^2$ in the quantum case).[24]

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HIT THAT DESK, SOLDIER!

In American parlance the expression ''basic training'' refers to the instruction given to recruits in the armed forces. Its purpose is to ensure that the trainees emerge with the fitness that will be expected of them when they embark on their main mission ...

But this course is *unlike* a boot camp in that you will not be asked to do things without question; no instructor will bark at you to ''hit that desk and given me fifty derivatives of e^x.'' You are encouraged to question everything, and as far as possible everything you do will be given a logical explanation and motivation.

The course *will be* like a boot camp in that you will be expected to work hard and struggle often, and will emerge proud of your mathematical fitness.

R. Shankar, *Basic Training in Mathematics—A Fitness Program for Science Students* (Plenum Press, New York, 1995), p. xi.