

Chapter 14

Propagation of Non-Gaussian Wave-Packets in Two Dimensions

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14.1 Introduction

Wave-packet dynamics can be realised in various physical systems. For example, in cold atom physics wave-packets can be used to model the motion of matter waves [1] or model electron packets in the dynamics of Rydberg atoms [2]. In quantum chemistry wave-packets are used to model chemical processes [3, 4]. When modelling physical systems it is very useful to look for analytic solutions as these can provide significant insight into the behaviour of the system and allow for general predictions to be made. However, there are many cases in which it becomes impossible to find a general analytic solution. In these scenarios numerical methods can be applied to model systems through solving differential equations numerically. Early analysis of systems with time-dependent potentials includes charged particles in electromagnetic fields [5] and 2D wave-packets in magnetic fields [6]. In this Chapter we present a procedure to analytically propagate *non*-Gaussian wave-packets in two dimensions. This builds upon the semi-classical dynamics of Heller [7], essentially a Gaussian wave-packet propagation, and the theory of “extended wave-packet propagation” originally formulated for one-dimension [8]. A series of transformations of the Schrödinger equation, including rotation in 2D, are used to derive the time evolution in a local basis. Of course, two dimensional quantum systems allow the inclusion of angular momentum which can be divided into both internal and external angular momentum and a study has been made for the special case of Gaussian wave packets in Ref. [9] with a general formalism presented in Ref. [10].

As a concrete example we will focus on matter-wave wave-packets and approximations to their dynamics. One such semi-classical method is an approach given by Heller [7]. The details of this method will be outlined in subsection 14.2.1 but in short, it uses a Gaussian wave-packet ansatz to generate a system of ordinary differential equations that can be solved to provide the time evolution. This solution will be an approximate one due to making a second order approximation of the potential. However, a method exists to systematically add corrections to the approximate solution. This is known as “Extended Gaussian Wave-Packet Dynamics” [8] and works by isolating the time evolution that comes from the higher order terms in the potential the Heller approach neglects. This additional time evolution is added back into the solution by solving additional differential equations. This allows for non-Gaussian wave-packets to be propagated, to a certain level of accuracy, in the same way as the normal Gaussian Heller wave-packets.

The benefit of the Heller method is that the time evolution of a wave-packet can be found through the solving of a system of first order differential equations. This is usually less computationally intensive than direct solving algorithms such as the split-step Fourier method [11] which requires position space to be discretised. This becomes ever more computationally intensive as more dimensions are added to the system being studied. Therefore, the Heller method offers a more efficient alternative.

When using the Heller method in one dimension corrections can be added to the approximate solution using the extended Gaussian wave-packet approach [8]. However, no such method existed for more dimensions, and thus the Heller method can provide inaccurate solutions in such cases. As an example we will consider the Heller method being applied to a wave-packet propagating in a two-dimensional ring trap. A harmonic ring trap in two dimensions will have a confining potential

$$V(r) = \frac{1}{2}m\omega^2(r - r_0)^2, \quad (14.1)$$

where ω is the angular frequency of the trap and r_0 is the radius of the ring. This potential is then used to propagate a Heller wave-packet, the details of which being given in section 14.2.2. A comparison between the Heller method and the split-step method is displayed in figure 14.1 where we find that the final positions and velocities are the same for both wave-packets indicating that the centre of mass motion is being appropriately accounted for by the Heller method. As expected the wave-packets in both methods have spread in space as the time evolution is carried out, however, there are distinct differences between the way in which they have spread. In the split-step method the wave-packet has spread around the ring itself, whereas the spreading in the Heller method is tangential to the ring. This discrepancy is a result of using the Heller wave-packet ansatz where there can be no curvature in the wave-packet. This lack of curvature is the feature that can be corrected by furthering the extended Gaussian wave-packet method allowing it to work in higher dimensions. Thus, in the following we will detail how the the method is extended to two dimensions.

In the next Section 14.2 we will first outline the Heller approach in one and two dimensions (sections 14.2.1 and 14.2.2 respectively). This introduces the basic method before introducing the extended Gaussian wave-packet approach in section 14.2.3. This approach will provide corrections in one dimension, which will guide the calculations in the rest of the study. Section 14.3 covers the series of transformations that need to

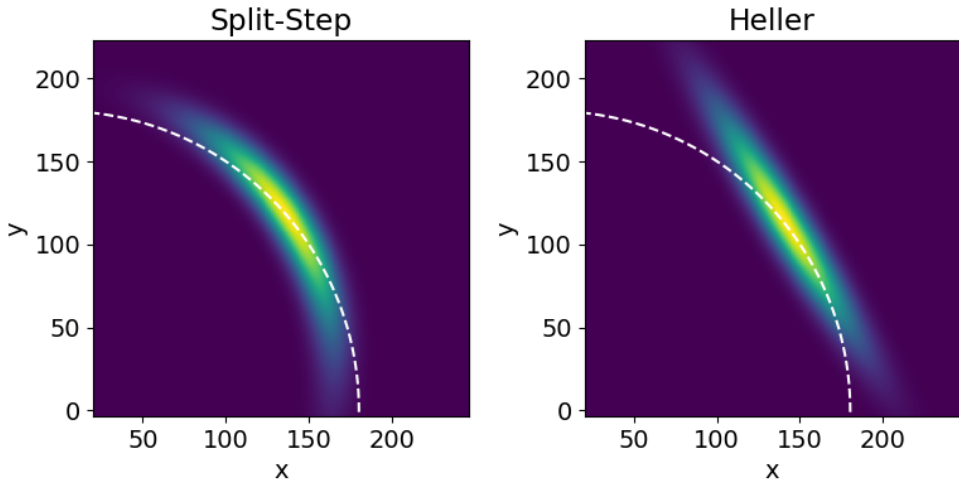


Figure 14.1: The position of a wave-packet is shown after it has made a complete rotation around the ring system and then evolved further in time. The position is compared using two numerical methods: the split-step numerical method [11] and the Heller method (Sec. 14.2.2). The parameters for this simulation in scaled units (described in 14.5) are: $m = 1$, $\hbar = 1$, $x_{lim} = 250$, $\Delta x = \Delta y = 0.5$, $r_0 = 125$, $\omega = 0.01$, $v_y(0) = 1$, $r'_0 = 180$, $t_f = 200\pi$ and $\Delta t = \pi/4$. The central position of the wave-packets can be seen to be the same but the way that they spread in space is distinctly different. In the split-step method there is a curving of the wave-packet around the ring that is not present in the Heller method.

be made to the Schrödinger equation in order to preform the extended Gaussian wave-packet propagation in two dimensions. The sections 14.3.1–14.3.5 will each cover a specific transformation that is made, examining its application and resulting equation. Section 14.3.1 deals with the selection of the centre of mass frame while section 14.3.2 covers a change of phase of the system. The addition of a second dimension introduces a new “ xy ” term which needs to be removed via a rotation transformation which we perform in two steps. In the first step, Section 14.3.3, we apply a first rotation to the principal axes of the local potential. This rotation produces an angular momentum term which is removed by the fuller transformation in the following section 14.3.4. Finally, the section 14.3.5 introduces the squeezing transformation that is applied in both the x and y direction to isolate the time evolution that comes from the residual potential. This results in the correct transformations being found to propagate a non-Gaussian wave-packet in two dimensions. The Chapter concludes in Sec. 14.4 and with the two appendices 14.5 and 14.6 which provide information on the scaling system used and details of the angular momentum calculation for the Heller semi-classical wave-packet.

14.2 Modelling Wave-Packet Dynamics

14.2.1 Heller Method in 1D

To demonstrate the use of Heller-wave packet dynamics in simulating the motion of matter waves we will first look at how the method works in one dimension. The general principle of the method is to assume a Gaussian wave-packet ansatz that is dependent on parameters that describe the key properties of the wave-packet, such as the centre of mass. This ansatz can then be substituted into the Schrödinger equation to find differential equations describing the time evolution of these parameters. Then by solving these differential equations the motion of the wave-packet is known. The specific Gaussian wave-packet ansatz used is given by

$$\psi(x, t) = \exp \left\{ \frac{i}{\hbar} [\alpha_t(x - x_t)^2 + p_t(x - x_t) + \gamma_t] \right\}, \quad (14.2)$$

where $\alpha(t) \equiv \alpha_t$ is a complex parameter describing the spreading, x_t is the central position of the wave-packet, p_t the central momentum and γ_t a complex phase factor that contains the normalisation. Note that the width of the wave-packet is contained within the imaginary part of $\alpha(t)$.

The wave-packet ansatz (14.2) can be substituted into the Schrödinger equation and coefficients matched, in order to determine the differential equations that describe the time evolution of the parameters x_t, p_t, α_t and γ_t . In order to match coefficients and derive first order differential equations an approximation to the potential needs to be made. This is carried out by Taylor expanding the potential and then neglecting terms higher than second order in x . With this approximation to the potential made, the *approximate* 1D Hamiltonian will be given by

$$H(x, t) = -\frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} + V(x_t) + \frac{\partial V}{\partial x}(x - x_t) + \frac{1}{2} \frac{\partial^2 V}{\partial x^2}(x - x_t)^2, \quad (14.3)$$

where the Taylor expansion has been carried out about a point $x = x_t$ i.e. the centre of the wave-packet. The derivatives of the potential are taken at this point $x = x_t$ but this has not been explicitly stated in the above expression for simplicity. Substituting the ansatz (14.2) and Hamiltonian (14.3) into the Schrödinger equation allows for the derivation of a system of differential equations governing the motion of the wave-packets. This is carried out by comparing coefficients of $(x - x_t)$ and isolating parameters x_t, p_t, α_t and γ_t giving the differential equations [7]:

$$\frac{dx_t}{dt} = \frac{\partial H(x_t, t)}{\partial p_t}, \quad (14.4)$$

$$\frac{dp_t}{dt} = -\frac{\partial H(x_t, t)}{\partial x_t}, \quad (14.5)$$

$$\frac{d\alpha_t}{dt} = -\frac{2}{m} \alpha_t^2 - \frac{1}{2} \frac{\partial^2 V}{\partial x^2}, \quad (14.6)$$

$$\frac{d\gamma_t}{dt} = i \frac{\hbar}{m} \alpha_t + \frac{p_t^2}{2m} - V(x_t, t). \quad (14.7)$$

The first two equations (14.4, 14.5) are the standard classical Hamiltonian equations of motion [12], indicating these classical trajectories accurately describe the centre of mass

motion of the wave-packet. Another interesting point is that the spreading of the wave-packet is only affected by terms in the potential of second order, therefore any linear or zeroth order potentials will only change the phase and motion of the wave-packet. There are two parts to the differential equation governing the time evolution of γ_t (14.7), the first is the correction to the normalisation that comes from the spreading of the wave-packet while the second can be recognised to be the Lagrangian. Thus, the phase factor will be dependent on the action along the trajectory as is expected from the path integral approach [13].

The above equations (14.4-14.7) can be solved for a given Hamiltonian and the solutions substituted into the wave-packet ansatz (14.2) to find the time evolution of the wave-packet. In some systems this can be carried out analytically, however, in the case where this is not possible numerical methods can be used to find the solutions instead [14].

14.2.2 Heller Method in 2D

The Heller approach can be extended to higher dimensions by following the same general steps but applied to each orthogonal direction involved [7]. First, the Hamiltonian will be expanded around a time-dependent point (x_t, y_t) and terms higher than second order are again neglected

$$\begin{aligned}
 H(x, y, t) = & -\frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} + -\frac{\hbar}{2m} \frac{\partial^2}{\partial y^2} + V(x_t, y_t, t) + (x - x_t) \frac{\partial V}{\partial x} + (y - y_t) \frac{\partial V}{\partial y} \\
 & + \frac{1}{2}(x - x_t)^2 \frac{\partial^2 V}{\partial x^2} + \frac{1}{2}(y - y_t)^2 \frac{\partial^2 V}{\partial y^2} + (x - x_t)(y - y_t) \frac{\partial^2 V}{\partial x \partial y}. \quad (14.8)
 \end{aligned}$$

As a reminder, the derivatives of the potential are evaluated at the time-dependent point $(x = x_t, y = y_t)$ in Eq. (14.8). The presence of this xy term will change the wave-packet ansatz since in addition to spreading in the x and y directions an xy term is needed to fully capture the dynamics. Then the new two dimensional wave-packet ansatz is

$$\begin{aligned}
 \psi(x, y, t) = \exp \left\{ \frac{i}{\hbar} [\alpha_x (x - x_t)^2 + \alpha_y (y - y_t)^2 + \lambda_t (x - x_t)(y - y_t) \right. \\
 \left. + p_x (x - x_t) + p_y (y - y_t) + \gamma_t \right\}. \quad (14.9)
 \end{aligned}$$

The parameters (x_t, y_t) give the central position of the wave-packet, (p_x, p_y) give the centre of momentum, (α_x, α_y) give the spreading in the directions indicated by the subscript, λ_t is a new complex parameter governing the spreading in the xy direction and γ_t is still a phase factor.

As with the one dimensional calculation, the wave-packet ansatz (14.9) and the approximate potential (14.8) are substituted into the Schrödinger equation to produce differential

equations for the parameters $(x_t, y_t, p_x, p_y, \alpha_x, \alpha_y, \lambda_t, \gamma_t)$:

$$\frac{dx_t}{dt} = \frac{\partial H(x_t, y_t, t)}{\partial p_x}, \quad (14.10)$$

$$\frac{dy_t}{dt} = \frac{\partial H(x_t, y_t, t)}{\partial p_y}, \quad (14.11)$$

$$\frac{dp_x}{dt} = -\frac{\partial H(x_t, y_t, t)}{\partial x_t}, \quad (14.12)$$

$$\frac{dp_y}{dt} = -\frac{\partial H(x_t, y_t, t)}{\partial y_t}, \quad (14.13)$$

$$\frac{d\lambda}{dt} = -2\frac{\lambda}{m}(\alpha_x + \alpha_y) - \frac{\partial V}{\partial x \partial y}, \quad (14.14)$$

$$\frac{d\alpha_x}{dt} = -\frac{2}{m}\alpha_x^2 - \frac{1}{2}\frac{\partial^2 V}{\partial x^2} - \frac{\lambda^2}{2m}, \quad (14.15)$$

$$\frac{d\alpha_y}{dt} = -\frac{2}{m}\alpha_y^2 - \frac{1}{2}\frac{\partial^2 V}{\partial y^2} - \frac{\lambda^2}{2m}, \quad (14.16)$$

$$\frac{d\gamma_t}{dt} = i\frac{\hbar}{m}\alpha_x + i\frac{\hbar}{m}\alpha_y + \frac{p_x^2}{2m} + \frac{p_y^2}{2m} - V(x_t, y_t, t). \quad (14.17)$$

This system of ordinary differential equations can be solved for a specific Hamiltonian and the solutions substituted into the wave-packet ansatz (14.9) to find the time evolution of the wave-function.

14.2.3 Extended Gaussian Wave-Packets

Unlike the physical wave-packets, when a Heller wave-packet propagates in the example ring trap its shape does not change as was shown in figure 14.1. The origin of this is understood to be the approximation made to the potential (14.3) as part of the derivation of the Heller equations. Since the approximated potential discards any terms higher than second order it allows for the Heller equations to be derived such that the solutions satisfy the initial Gaussian ansatz (14.2). While this approximation allows for the method to work, it limits the shape of the wave-packet to be exactly a Gaussian shape since any changes to this shape would come from the higher order terms.

The limitation to the shape of the wave-packet has been observed and mitigated in *one dimensional* problems with the use of “extended Gaussian wave-packet dynamics” [8]. This general method takes the Heller approach as a basis and systematically adds in the effects of the higher order terms. This is carried out by first isolating the evolution of the wave-packet that comes solely from the higher order terms by repeatedly transforming the Schrödinger equation. The final form of this will be (in units where $\hbar = 1$ and $m = 1$

here on)

$$\begin{aligned}
 i\frac{\partial\psi(x,t)}{\partial t} &= \left[\frac{\hat{p}^2}{2} + V(x) \right] \psi(x,t), \\
 &= \left[\frac{\hat{p}^2}{2} + V(0) + x\frac{\partial V(0)}{\partial x} + x^2\frac{1}{2}\frac{\partial^2 V(0)}{\partial x^2} + \dots \right] \psi(x,t), \\
 \rightarrow i\frac{\partial\psi'(x,t)}{\partial t} &= \left[\frac{1}{3!}\frac{x^3\partial^3 V(0)}{\partial x^3} + x^4\frac{1}{4!}\frac{\partial^4 V(0)}{\partial x^4} + \dots \right] \psi'(x,t), \\
 &= V_R(x)\psi'(x,t),
 \end{aligned} \tag{14.18}$$

where $\psi'(x,t)$ is the wave-function that has had a series of transformations applied to it and $V_R(x)$ is the residual potential containing the terms the Heller approach neglects. In this one dimensional case these transformations are: a displacement, a change of phase and a time dependent squeezing operation. Through these transformations a non-Gaussian wave-packet can be propagated in the same way as the Heller wave-packets. In practice this is achieved by going to the Fock basis and finding matrix elements of V_R . This method works since these matrix elements determine the time evolution of the higher energy $|n\rangle$ states which are neglected by the Heller approach. The result of this is that the higher energy states can be accounted for through additional differential equations that can be solved in parallel with the Heller equations. To find the propagation of N additional states it requires solving $6 + 2N$ linear first order differential equations [8]. In practice the number of additional states chosen determines the accuracy of the numerical simulations, with more states giving a more accurate result subject to diminishing returns.

Generalising this approach to two dimensions will allow for the deformation in shape seen in figure 14.1 to be accounted for numerically by solving a finite number of differential equations. This will save time on making intensive computations using direct solvers. The approach for generalising to two dimensions can be used as part of future work to generalise further, describing the motion of three dimensional wave-packets.

14.3 Transformations

Now that the general approach for using extended Gaussian wave-packets has been outlined in 1D, it can be used as a basis for the two dimensional version. In a similar way we will isolate the residual potential by continually transforming the Schrödinger equation to remove harmonic terms. This will closely follow the one dimensional version but repeating the steps in both the x and y direction. There will be one new cross-term that depends on xy which can be removed by making the correct rotation.

To start the calculation we first need the Schrödinger equation that describes the time evolution of a two dimensional wave function. This Schrödinger equation will be put into a form where the potential is expanded similarly to equations (14.18). The two

dimensional Schrödinger equation in this form can be expressed as

$$i \frac{\partial \Psi(x, y, t)}{\partial t} = \left[\frac{\hat{p}_x^2}{2} + \frac{\hat{p}_y^2}{2} + V_0 + (\hat{x} - x_t)V_x + (\hat{y} - y_t)V_y \right. \\ \left. + (\hat{x} - x_t)^2 \frac{V_{xx}}{2} + (\hat{y} - y_t)^2 \frac{V_{yy}}{2} \right. \\ \left. + (\hat{x} - x_t)(\hat{y} - y_t)V_{xy} + V_R(\hat{x}, \hat{y}) \right] \Psi(x, y, t), \quad (14.19)$$

where the subscript of the potentials indicate the derivatives taken, with each being evaluated at the point $x = x_t$, $y = y_t$. The residual potential V_R contains all the higher order terms similar to the one defined in the one dimensional version (14.18). If the residual potential is removed then we obtain the Schrödinger equation used by Heller for the propagation of wave-packets. Therefore, removing all the harmonic terms isolates only the effects from terms the Heller approach neglects. These terms are removed by transforming the wave-function and Hamiltonian with the appropriate operators. The following calculation will go through each transformation of the Schrödinger equation systematically until all the terms other than $V_R(\hat{x}, \hat{y})$ have been removed. Doing this will allow for wave-packets of a non Gaussian shape to be propagated.

14.3.1 Displacement

Following the same approach as the one dimensional problem, the first transformation that will be made is a displacement of the wave-function to bring it into the centre of mass frame i.e. centred around x_t, y_t, p_x, p_y . The goal of this transformation is to remove any terms in the Hamiltonian that depend linearly on $\hat{x}, \hat{y}, \hat{p}_x, \hat{p}_y$. This displacement transformation is made in a single spatial direction by the displacement operator given by [15]

$$\hat{D}(x_t, p_x) = \exp[i(p_x \hat{x} - x_t \hat{p}_x)], \quad (14.20)$$

with its inverse transformation being

$$\hat{D}^{-1}(x_t, p_x) = \hat{D}(-x_t, -p_x). \quad (14.21)$$

This operator displaces a general function $U(\hat{x}, \hat{p})$ as

$$\hat{D}^{-1}(x_t, p_x)U(\hat{x}, \hat{p})\hat{D}(x_t, p_x) = U(\hat{x} + x_t, \hat{p} + p_x). \quad (14.22)$$

This operator can be applied to the wave-function to shift the co-ordinate system to the centre of mass so that the origin becomes $x_0 = x_t$, $v_0 = v_t$ in position space and similarly in momentum space. The relation of this new displaced wave-function $\psi_d(x, y, t)$ to the initial wave-function is

$$\psi_d(x, y, t) = \hat{D}_x^{-1}(x_t, p_x)\hat{D}_y^{-1}(y_t, p_y)\Psi(x, y, t). \quad (14.23)$$

This relation can be utilized in the Schrödinger equation (14.19) to find the time evolution of $\psi_d(x, y, t)$. This is carried out by multiplying the equation from the left by $\hat{D}^{-1}(x_t, p_x)\hat{D}^{-1}(y_t, p_y)$ after the substitution has been made. Doing so isolates a term with the time derivative of the displaced wave-function

$$\begin{aligned}
 i \frac{\partial \psi_d(x, y, t)}{\partial t} = & \left[\frac{(\hat{p}_x + p_x)^2}{2} + \frac{(\hat{p}_y + p_y)^2}{2} + V_0 + \hat{x}V_x + \hat{y}V_y \right. \\
 & + \hat{x}^2 \frac{V_{xx}}{2} + \hat{y}^2 \frac{V_{yy}}{2} + \hat{x}\hat{y}V_{xy} + V_R(\hat{x} + x_t, \hat{y} + y_t) \\
 & \left. - i\hat{D}_x^{-1} \left(\frac{\partial \hat{D}_x}{\partial t} \right) - i\hat{D}_y^{-1} \left(\frac{\partial \hat{D}_y}{\partial t} \right) \right] \psi_d(x, y, t). \quad (14.24)
 \end{aligned}$$

This transformation has displaced the wave-function and operators but it has also generated two terms that are dependent on the derivatives of the displacement operator. The derivatives can be taken and simplified by substituting in the classical Hamiltonian equations of motion [12]:

$$\begin{aligned}
 -i\hat{D}^{-1}(x_t, p_x) \left(\frac{\partial \hat{D}(x_t, p_x)}{\partial t} \right) &= -i\hat{D}^{-1}(x_t, p_x) \hat{D}(x_t, p_x) \frac{\partial}{\partial t} (ip_x \hat{x} - ix_t \hat{p}_x), \\
 &= \frac{\partial p_x}{\partial t} \hat{x} - \frac{\partial x_t}{\partial t} \hat{p}_x, \\
 &= -V_x \hat{x} - p_x \hat{p}_x. \quad (14.25)
 \end{aligned}$$

Substituting in this result, as well as the corresponding one for the y direction, into equation (14.24) removes all the linear terms from the Hamiltonian

$$\begin{aligned}
 i \frac{\partial \psi_d(x, y, t)}{\partial t} = & \left[V_0 + \frac{p_x^2}{2} + \frac{p_y^2}{2} + \frac{\hat{p}_x^2}{2} + \frac{\hat{p}_y^2}{2} \right. \\
 & \left. + \hat{x}^2 \frac{V_{xx}}{2} + \hat{y}^2 \frac{V_{yy}}{2} + \hat{x}\hat{y}V_{xy} + V_R(\hat{x} + x_t, \hat{y} + y_t) \right] \psi_d(x, y, t). \quad (14.26)
 \end{aligned}$$

With this transformation being made, the form of the Schrödinger equation is brought closer to one in which the only remaining term in the Hamiltonian is the residual potential. This general process of transforming the wave-function and the Hamiltonian to remove terms will be repeated throughout the following calculation.

14.3.2 Change of Phase

The next terms we remove from equation (14.26) are the zeroth order terms. This can be achieved by multiplying the wave-function by a time dependent phase factor. The new wave-function $\psi_{dp}(x, y, t)$ is related to the old wave-function (14.23) by

$$\psi_{dp}(x, y, t) = \exp[i\phi(t)] \psi_d(x, y, t), \quad (14.27)$$

where the phase $\phi(t)$ in the above expression is given by

$$\phi(t) = \int_0^t \left[V_0(x_{t'}, y_{t'}) + \frac{p_x(t')^2}{2} + \frac{p_y(t')^2}{2} \right] dt'. \quad (14.28)$$

The terms in this integral have been chosen to be exactly the zeroth order terms that we wish to remove by making this transformation. When the above expression is substituted into the Schrödinger equation it will cancel the non-operator terms

$$\begin{aligned}
 i \frac{\partial \psi_{dp}(x, y, t)}{\partial t} &= \left[\frac{\hat{p}_x^2}{2} + \frac{\hat{p}_y^2}{2} + \frac{p_x^2}{2} + \frac{p_y^2}{2} + V_0 + \hat{x}^2 \frac{V_{xx}}{2} + \hat{y}^2 \frac{V_{yy}}{2} + \hat{x}\hat{y}V_{xy} \right. \\
 &\quad \left. + V_R(\hat{x} + x_t, \hat{y} + y_t) - \frac{\partial \phi(t)}{\partial t} \right] \psi_{dp}(x, y, t), \\
 &= \left[\frac{\hat{p}_x^2}{2} + \frac{\hat{p}_y^2}{2} + \hat{x}^2 \frac{V_{xx}}{2} + \hat{y}^2 \frac{V_{yy}}{2} + \hat{x}\hat{y}V_{xy} + V_R(\hat{x} + x_t, \hat{y} + y_t) \right] \psi_{dp}(x, y, t).
 \end{aligned} \tag{14.29}$$

Thus, the zeroth order terms have been removed. The next set of transformations will deal with removing the second order terms from the Schrödinger equation.

14.3.3 Principal Axes Rotation

In the one dimensional extended Gaussian wave-packet approach the second order terms are removed from the Hamiltonian via a time dependent squeezing operator. However, there is a distinct difference in the Schrödinger equation (14.29) namely, there is the presence of an xy term. If this term were to be removed then the rest of the calculation will closely resemble that of the one dimensional problem but repeated twice for both the x and y directions.

The xy term in the transformed Schrödinger equation (14.29) can be removed by a principal axis rotation. This will create new coefficients for the x^2 and y^2 terms but remove the xy term completely. If we rotate the co-ordinates by an angle θ then the new co-ordinates (x', y') can be expressed in terms of the old co-ordinates (x, y) as [16]

$$x' = x \cos(\theta) + y \sin(\theta), \tag{14.30}$$

$$y' = y \cos(\theta) - x \sin(\theta). \tag{14.31}$$

Next we will examine how these transformed co-ordinates affect the potential $V(x, y) = x^2 V_{xx} + y^2 V_{yy} + xy V_{xy}$, since this potential resembles the terms in equation (14.29). In full these coefficients V_{xx} , V_{yy} and V_{xy} are going to be time dependent due to being evaluated at a point (x_t, y_t) . The result of this time dependence is that the rotation angle will also be time dependent. The potential can be rotated and expressed in terms of the old co-ordinate system by substituting the relations (14.30, 14.31) and collecting like terms:

$$\begin{aligned}
 V(x', y') &= [x \cos(\theta) + y \sin(\theta)]^2 V_{xx} + [y \cos(\theta) - x \sin(\theta)]^2 V_{yy} \\
 &\quad + [x \cos(\theta) + y \sin(\theta)] [y \cos(\theta) - x \sin(\theta)] V_{xy}, \\
 &= \{V_{xx} \cos^2(\theta) - V_{xy} \cos(\theta) \sin(\theta) + V_{yy} \sin^2(\theta)\} x^2 \\
 &\quad + \{V_{yy} \cos^2(\theta) + V_{xy} \cos(\theta) \sin(\theta) + V_{xx} \sin^2(\theta)\} y^2 \\
 &\quad + \{V_{xy} [\cos^2(\theta) - \sin^2(\theta)] + 2[V_{xx} - V_{yy}] \sin(\theta) \cos(\theta)\} xy.
 \end{aligned} \tag{14.32}$$

The xy term can be eliminated by the correct choice of rotation angle θ such that the two terms in the last line of the above expression cancel. To find the expression for this angle we set a condition that the terms inside the bracket on the last line sum to zero i.e.

$$2[V_{yy} - V_{xx}] \sin(\theta) \cos(\theta) = V_{xy} [\cos^2(\theta) - \sin^2(\theta)], \quad (14.33)$$

$$2[V_{yy} - V_{xx}] \tan(\theta) = V_{xy} [1 - \tan^2(\theta)], \quad (14.34)$$

where the expression has been simplified by dividing both sides by $\cos^2(\theta)$. The angle can be found by rearranging the above expression and using a double angle formula for $\tan(2\theta)$

$$\theta(x_t, y_t) = \frac{1}{2} \arctan \left(\frac{V_{xy}(x_t, y_t)}{[V_{yy}(x_t, y_t) - V_{xx}(x_t, y_t)]} \right). \quad (14.35)$$

This angle of rotation will be dependent on time via the parameters x_t and y_t . When it is substituted into the potential (14.32) it can be rewritten as

$$V(x', y') = V'_{xx}x^2 + V'_{yy}y^2, \quad (14.36)$$

where the new coefficients are given by the quantities

$$V'_{xx} = V_{xx} \cos^2(\theta) - V_{xy} \cos(\theta) \sin(\theta) + V_{yy} \sin^2(\theta), \quad (14.37)$$

$$V'_{yy} = V_{yy} \cos^2(\theta) + V_{xy} \cos(\theta) \sin(\theta) + V_{xx} \sin^2(\theta). \quad (14.38)$$

Thus, the result of the rotation is that the xy term has been removed from the local potential.

To carry out this co-ordinate rotation for the whole system, not just the potential, the correct operator will be needed. This rotation operator is defined by [15]

$$\hat{U}_R(\theta) = \exp(-i\theta\hat{L}_z) = \exp[-i\theta(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x)]. \quad (14.39)$$

This can be used to rotate the co-ordinate system by applying the transformation to the operators \hat{x} , \hat{y} , \hat{p}_x and \hat{p}_y . By rotating through an angle θ the desired transformations of the operators are achieved:

$$\hat{x}' = \hat{U}_R(\theta)\hat{x}\hat{U}_R(-\theta) = \cos(\theta)\hat{x} + \sin(\theta)\hat{y}, \quad (14.40)$$

$$\hat{y}' = \hat{U}_R(\theta)\hat{y}\hat{U}_R(-\theta) = \cos(\theta)\hat{y} - \sin(\theta)\hat{x}, \quad (14.41)$$

$$\hat{p}'_x = \hat{U}_R(\theta)\hat{p}_x\hat{U}_R(-\theta) = \cos(\theta)\hat{p}_x + \sin(\theta)\hat{p}_y, \quad (14.42)$$

$$\hat{p}'_y = \hat{U}_R(\theta)\hat{p}_y\hat{U}_R(-\theta) = \cos(\theta)\hat{p}_y - \sin(\theta)\hat{p}_x, \quad (14.43)$$

where the results are calculated with the application of the Baker-Hausdorff lemma [17]. These transformations match the previous coordinate transformations in equations (14.30, 14.31) demonstrating that the rotation operator serves the desired function. Note that the above transformations can be used to show that the angular momentum operator \hat{L}_z is the same regardless of the angle of rotation chosen:

$$\begin{aligned} \hat{U}_R(\theta)\hat{L}_z\hat{U}_R(-\theta) &= (\cos(\theta)\hat{x} + \sin(\theta)\hat{y})(\cos(\theta) - \sin(\theta)\hat{p}_x) \\ &\quad - (\cos(\theta)\hat{y} - \sin(\theta)\hat{x})(\cos(\theta)\hat{p}_x + \sin(\theta)\hat{p}_y), \\ &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x. \end{aligned} \quad (14.44)$$

Thus, the operator will be the same in any new co-ordinate system x', y' .

As with the previous calculations, the wave-function (14.27) will need to be transformed alongside the transformation of the Hamiltonian. This is again achieved by the appropriate application of the inverse rotation operator so that

$$\psi_{dpr}(x, y, t) = \hat{U}_R^{-1}(-\theta(t))\psi_{dp}(x, y, t) = \hat{U}_R(\theta(t))\psi_{dp}(x, y, t). \quad (14.45)$$

The use of the the inverse rotation operator in this transformation is such that when the Hamiltonian is multiplied from the left by $U_R(\theta(x_t, y_t))$ the coordinates will be transformed according to equations (14.40-14.43). Substituting the new wave-function (14.45) into the Schrödinger equation (14.29), it is transformed as

$$\begin{aligned} i \frac{\partial \psi_{dpr}(x, y, t)}{\partial t} &= \hat{U}_R(\theta(t)) \hat{H} \hat{U}_R(-\theta(t)) \psi_{dpr}(x, y, t) \\ &\quad - i \hat{U}_R(\theta(t)) \left[\frac{\partial \hat{U}_R(-\theta(t))}{\partial t} \right] \psi_{dpr}(x, y, t), \end{aligned} \quad (14.46)$$

where the Hamiltonian \hat{H} is given by

$$\hat{H} = \frac{\hat{p}_x^2}{2} + \frac{\hat{p}_y^2}{2} + \hat{x}^2 \frac{V_{xx}}{2} + \hat{y}^2 \frac{V_{yy}}{2} + \hat{x} \hat{y} V_{xy} + V_R(\hat{x} + x_t, \hat{y} + y_t). \quad (14.47)$$

Since we want to know how the final term in (14.46) changes the Hamiltonian we will need to evaluate it. Computing the derivative and multiplying by the rotation operator gives

$$i \hat{U}_R(\theta(t)) \left(\frac{\partial \hat{U}_R(-\theta(t))}{\partial t} \right) = \frac{\partial \theta(t)}{\partial t} (\hat{x} \hat{p}_y - \hat{y} \hat{p}_x). \quad (14.48)$$

Using this result and gathering terms in equation (14.46) produces a new Schrödinger equation where the rotation has been carried out

$$\begin{aligned} i \frac{\partial \psi_{dpr}(x, y, t)}{\partial t} &= \left[\frac{\hat{p}_x^2}{2} + \frac{\hat{p}_y^2}{2} + \hat{x}^2 \frac{V'_{xx}}{2} + \hat{y}^2 \frac{V'_{yy}}{2} \right. \\ &\quad \left. + V_R(\hat{x}' + x_t, \hat{y}' + y_t) - \frac{\partial \theta(x_t, y_t)}{\partial t} (\hat{x} \hat{p}_y - \hat{y} \hat{p}_x) \right] \psi_{dpr}(x, y, t). \end{aligned} \quad (14.49)$$

The coefficients V'_{xx} and V'_{yy} are given by the same expressions as the ones derived for a simple co-ordinate transformation of the potential (14.37, 14.38). However, a rotation term depending on \hat{L}_z has been introduced which prevents a local separation of variables. In the next section, a full rotation is used to eliminate this angular momentum term.

14.3.4 Full Rotation

It has been shown in the previous section 14.3.3 that it is necessary to rotate the system not to where the xy term in the potential is zero but to a coordinate system where the xy term balances the new angular momentum term (14.48). To find what this other

co-ordinate system is, we examine the full form of the transformed Schrödinger equation (14.46) substituting in the result from equation (14.48):

$$\begin{aligned}
 i \frac{\partial \psi_{dpr}}{\partial t}(x, y, t) = & \left\{ \frac{\hat{p}_x^2}{2} + \frac{\hat{p}_y^2}{2} + \hat{x}^2 [V_{xx} \cos^2(\theta) - V_{xy} \cos(\theta) \sin(\theta) + V_{yy}] \right. \\
 & + \hat{y}^2 [V_{yy} \cos^2(\theta) + V_{xy} \cos(\theta) \sin(\theta) + V_{xx} \sin^2(\theta)] \\
 & + \hat{x} \hat{y} [V_{xy} (\cos^2(\theta) - \sin^2(\theta)) + 2(V_{xx} - V_{yy}) \sin(\theta) \cos(\theta)] \\
 & \left. - \frac{\partial \theta(x_t, y_t)}{\partial t} (\hat{x} \hat{p}_y - \hat{y} \hat{p}_x) + V_R(\hat{x}' + x_t, \hat{y}' + y_t) \right\} \psi_{dpr}(x, y, t). \quad (14.50)
 \end{aligned}$$

In order to gather like terms we can act on the wave-function with the angular momentum operator as given in 14.6 by equation (14.95)

$$(\hat{x} \hat{p}_y - \hat{y} \hat{p}_x) \psi_{dpr}(x, y, t) = (2(\alpha_y - \alpha_x)xy + \lambda x^2 + \lambda y^2) \psi_{dpr}(x, y, t), \quad (14.51)$$

where the parameters α_x, α_y and λ are the usual Heller parameters defined as part of the wave-packet ansatz (14.9). Thus, we can substitute this expression into the rotated Schrödinger equation (14.50) and gather terms by acting on the wave-function with the \hat{x} and \hat{y} operators

$$\begin{aligned}
 i \frac{\partial \psi_{dpr}(x, y, t)}{\partial t} = & \left\{ \frac{\hat{p}_x^2}{2} + \frac{\hat{p}_y^2}{2} + x^2 [V_{xx} \cos^2(\theta) - V_{xy} \cos(\theta) \sin(\theta) + V_{yy} \sin^2(\theta) - \frac{\partial \theta}{\partial t} \lambda] \right. \\
 & + y^2 [V_{yy} \cos^2(\theta) + V_{xy} \cos(\theta) \sin(\theta) + V_{xx} \sin^2(\theta) - \frac{\partial \theta}{\partial t} \lambda] \\
 & + xy [V_{xy} (\cos^2(\theta) - \sin^2(\theta)) + 2(V_{xx} - V_{yy}) \sin(\theta) \cos(\theta) - 2 \frac{\partial \theta}{\partial t} (\alpha_y - \alpha_x)] \\
 & \left. + V_R(\hat{x}' + x_t, \hat{y}' + y_t) \right\} \psi_{dpr}(x, y, t), \quad (14.52)
 \end{aligned}$$

where the time dependence of θ has not been explicitly stated for convenience. The xy term in the above expression will be eliminated by setting the condition that the coefficient is zero. Doing so gives a differential equation for the rotation angle

$$\frac{\partial \theta(t)}{\partial t} = \frac{1}{2(\alpha_y - \alpha_x)} \{ V_{xy} [\cos^2(\theta(t)) - \sin^2(\theta(t))] + 2 [V_{xx} - V_{yy}] \sin(\theta(t)) \cos(\theta(t)) \}. \quad (14.53)$$

This angle θ can be computed, along with its derivative, as part of the extended Gaussian wave-packet method. This will add additional differential equations that need to be solved as part of the method. This differential equation allows the Schrödinger equation (14.52) to be expressed as

$$i \frac{\partial \psi_{dpr}}{\partial t}(x, y, t) = \left[\frac{\hat{p}_x^2}{2} + \frac{\hat{p}_y^2}{2} + x^2 V'_{xx} + y^2 V'_{yy} + V_R(\hat{x}' + x_t, \hat{y}' + y_t) \right] \psi_{dpr}(x, y, t), \quad (14.54)$$

where the coefficients V'_{xx} and V'_{yy} are given by

$$V'_{xx} = V_{xx} \cos^2(\theta(t)) - V_{xy} \cos(\theta(t)) \sin(\theta(t)) + V_{yy} \sin^2(\theta(t)) - \frac{\partial\theta(t)}{\partial t} \lambda, \quad (14.55)$$

$$V'_{yy} = V_{yy} \cos^2(\theta(t)) + V_{xy} \cos(\theta(t)) \sin(\theta(t)) + V_{xx} \sin^2(\theta(t)) - \frac{\partial\theta(t)}{\partial t} \lambda. \quad (14.56)$$

Thus, we have transformed the Schrödinger equation into a frame where the rotation of the potential is exactly balanced by the angular momentum of the wave-packet. The xy term has been completely eliminated bringing the whole expression closer to one in which the residual potential is isolated.

14.3.5 Squeezing

Now that the coordinates have been rotated to a frame that eliminates any xy terms the system becomes a two dimensional harmonic oscillator with varying frequencies given by the coefficients V'_{xx} and V'_{yy} . Due to the rotation, these two axes are completely orthogonal allowing for each axis to be treated independently. This means that the calculation can closely resemble that of the one dimensional treatment [8]. The way the second order terms are removed in the one dimensional problem is by applying a time dependent squeezing operation therefore, in the two dimensional system we will apply a different time dependent squeezing to each axis simultaneously.

Time Dependent Two Dimensional Harmonic Oscillator and its Ground State

In order to calculate explicitly what the squeezing operation should be, we will first examine the two dimensional harmonic oscillator system in more detail. This will allow for notation to be introduced as well as to link the ground state of this system with the two dimensional Heller wave-packet ansatz. The Schrödinger equation for a two dimensional harmonic oscillator with time varying spring constants is given by

$$i \frac{\partial\psi(x, y, t)}{\partial t} = \left[\frac{\hat{p}_x^2}{2} + \frac{\hat{p}_y^2}{2} + x^2 k_x(t) + y^2 k_y(t) \right] \psi(x, y, t). \quad (14.57)$$

To find the “ground state” of this system we will follow the general process outlined in Ref. [18] but applied to two dimensions. The approach is to define a time dependent form of the creation and annihilation operator using constants of motion. Then the annihilation operator can be used to find the “ground state” for the system. This “ground state” will not be stationary since it will depend on time due to the explicit time dependence of the Hamiltonian. Since the state is not stationary it cannot be considered a true ground state. Since the new creation and annihilation operators are constants of motion, they can be applied in the two orthogonal directions simultaneously in much the same way as for a time independent harmonic oscillator. The time dependent annihilation operators will be defined for each direction as

$$\hat{A}_x(t) = \frac{i}{\sqrt{2}} [\epsilon_x(t) \hat{p}_x - \dot{\epsilon}_x(t) \hat{x}], \quad (14.58)$$

$$\hat{A}_y(t) = \frac{i}{\sqrt{2}} [\epsilon_y(t) \hat{p}_y - \dot{\epsilon}_y(t) \hat{y}], \quad (14.59)$$

where the ϵ functions are solutions to the classical differential equations

$$\ddot{\epsilon}_x(t) = -k_x(t)\epsilon_x(t), \quad (14.60)$$

$$\ddot{\epsilon}_y(t) = -k_y(t)\epsilon_y(t). \quad (14.61)$$

Here the dot notation is being used to specify a time derivative of the quantity e.g. $\dot{\epsilon}_x(t) = \partial\epsilon_x(t)/\partial t$. The $\epsilon_x(t)$, $\epsilon_y(t)$ solutions will guarantee that the operators $\hat{A}_x(t)$, $\hat{A}_y(t)$ are constants of motion. This can be demonstrated by taking the time derivative of the operators and seeing that this time derivative is zero. This will be shown first for the $\hat{A}_x(t)$ operator using the Hamiltonian given in equation (14.57)

$$\begin{aligned} \frac{d\hat{A}_x(t)}{dt} &= i \left[\hat{H}(t), \hat{A}_x(t) \right] + \frac{\partial\hat{A}_x(t)}{\partial t}, \\ &= \frac{\dot{\epsilon}_x(t)}{2\sqrt{2}} [\hat{p}_x^2, \hat{x}] - \frac{k_x(t)\epsilon_x(t)}{2\sqrt{2}} [\hat{x}^2, \hat{p}_x] + \frac{i}{\sqrt{2}}\dot{\epsilon}_x(t)\hat{p}_x - \frac{i}{\sqrt{2}}\ddot{\epsilon}_x(t)\hat{x}, \\ &= -\frac{i}{\sqrt{2}}(k_x(t)\epsilon_x(t) + \ddot{\epsilon}_x(t))\hat{x}. \end{aligned} \quad (14.62)$$

Thus, with the application of equation (14.60) it can be seen that the time derivative of the $\hat{A}_x(t)$ operator is zero and therefore, is a constant of motion. A similar calculation can be carried out to prove the same thing for $\hat{A}_y(t)$.

We will now demonstrate that with an appropriate choice of initial conditions the operators $\hat{A}_x(t)$ and $\hat{A}_y(t)$ will obey the familiar creation and annihilator operator commutation relations. Furthermore, this commutation relation will be time independent and thus, a ‘‘ground state’’ of the Hamiltonian can be defined [18]. The initial conditions for $\epsilon_x(t)$, $\epsilon_y(t)$, are set such that

$$\begin{aligned} \epsilon_x(0) = 1, \quad \dot{\epsilon}_x(0) = i, \quad &\implies \hat{A}_x(0) = \frac{1}{\sqrt{2}} [\hat{x} + i\hat{p}_x], \\ \epsilon_y(0) = 1, \quad \dot{\epsilon}_y(0) = i, \quad &\implies \hat{A}_y(0) = \frac{1}{\sqrt{2}} [\hat{y} + i\hat{p}_y]. \end{aligned} \quad (14.63)$$

The form of $\hat{A}_j(0)$, for $j = \{x, y\}$, is the same as the normal annihilation operator for a time-independent harmonic oscillator. The commutation relation for $\hat{A}_j(t)$ is

$$[\hat{A}_j(t), \hat{A}_j^\dagger(t)] = 1, \quad (14.64)$$

and it is zero for $[\hat{A}_x(t), \hat{A}_y^\dagger(t)]$. These results are found by applying the definition of the operators (14.58, 14.59), then at time $t = 0$ the initial conditions (14.63) give the above result that the commutation relation is one. It can then be shown by taking the derivative that the commutator does not change in time thus, it will always have a value of one.

Now that the properties of the operators $\hat{A}_x(t)$ and $\hat{A}_y(t)$ have been understood, they can be applied to find a ground state wave-function for the time dependent harmonic oscillator. Since the annihilation and creation operators in each direction commute with one another and the commutator (14.64) is time independent, it is possible to define number states $|n_x, n_y, t\rangle$ similar to those of the time independent harmonic oscillator [18]. The ‘‘ground state’’ will be defined by the relation

$$\hat{A}_x(t)\hat{A}_y(t)|0, 0, t\rangle = 0. \quad (14.65)$$

Since $\hat{A}_x(t)$ and $\hat{A}_y(t)$ commute they will act on $|n_x\rangle$ and $|n_y\rangle$ independently leading to two differential equations in the position space representation

$$\frac{-i}{\sqrt{2}} \left[i\epsilon_x(t) \frac{d}{dx} + \dot{\epsilon}_x(t)x \right] \psi_0(x, t) = 0, \quad (14.66)$$

$$\frac{-i}{\sqrt{2}} \left[i\epsilon_y(t) \frac{d}{dy} + \dot{\epsilon}_y(t)y \right] \psi_0(y, t) = 0, \quad (14.67)$$

where the “ground state” wave-function $\psi_0(x, y, t)$ is separated as $\psi_0(x, y, t) = \psi_0(x, t)\psi_0(y, t)$. The solution to these differential equations gives the “ground state”

$$\psi_0(x, y, t) = \frac{1}{\sqrt{\pi|\epsilon_x(t)||\epsilon_y(t)|}} \exp \left(\frac{i}{2} \frac{\dot{\epsilon}_x(t)}{\epsilon_x(t)} x^2 + \frac{i}{2} \frac{\dot{\epsilon}_y(t)}{\epsilon_y(t)} y^2 \right). \quad (14.68)$$

The above expression is the full position space representation of the ground state wave-function for the two dimensional time dependent harmonic oscillator. This has the form of a two dimensional Gaussian wave-packet and can be connected to the Heller wave-packet by performing the inverse transformations of ψ_{dpr} as detailed by equation (14.45):

$$\begin{aligned} \psi(x, y, t) &= \hat{D}_y(y_t, y_x) \hat{D}_x(x_t, p_x) e^{-i\phi(t)} \hat{U}(-\theta(t)) \psi_0(x, y, t), \\ &= \exp \left\{ \frac{i}{2} \left[\frac{\dot{\epsilon}_x}{\epsilon_x} \cos^2(\theta) + \frac{\dot{\epsilon}_y}{\epsilon_y} \sin^2(\theta) \right] (x - x_t)^2 + ip_x(x - x_t) \right. \\ &\quad + \frac{i}{2} \left[\frac{\dot{\epsilon}_y}{\epsilon_y} \cos^2(\theta) + \frac{\dot{\epsilon}_x}{\epsilon_x} \sin^2(\theta) \right] (y - y_t)^2 + ip_y(y - y_t) \\ &\quad \left. + i \left[\frac{\dot{\epsilon}_y}{\epsilon_y} - \frac{\dot{\epsilon}_x}{\epsilon_x} \right] \cos(\theta) \sin(\theta) (x - x_t)(y - y_t) - i\phi + \frac{i}{2} \ln(\pi|\epsilon_x||\epsilon_y|) \right\}, \end{aligned} \quad (14.69)$$

where the explicit time dependencies of the parameters $\epsilon_x, \epsilon_y, \theta, x_t, p_x, y_t, p_y$ and ϕ have not been explicitly stated for simplicity.

A direct comparison between the above expression and the regular form of the two dimensional Heller wave-packet (14.9) can be made. Coefficients can be compared to see that the two wave-functions have the same form with the Heller parameters being given by:

$$\alpha_x(t) = \frac{1}{2} \left[\frac{\dot{\epsilon}_x}{\epsilon_x} \cos^2(\theta) + \frac{\dot{\epsilon}_y}{\epsilon_y} \sin^2(\theta) \right], \quad (14.70)$$

$$\alpha_y(t) = \frac{1}{2} \left[\frac{\dot{\epsilon}_y}{\epsilon_y} \cos^2(\theta) + \frac{\dot{\epsilon}_x}{\epsilon_x} \sin^2(\theta) \right], \quad (14.71)$$

$$\lambda(t) = \left[\frac{\dot{\epsilon}_y}{\epsilon_y} - \frac{\dot{\epsilon}_x}{\epsilon_x} \right] \cos(\theta) \sin(\theta), \quad (14.72)$$

$$\gamma(t) = -\phi + \frac{i}{2} \ln \pi |\epsilon_x| |\epsilon_y|. \quad (14.73)$$

Therefore, we have found that the “ground state” of the two dimensional harmonic oscillator with time dependent spring constants corresponds directly to a Heller wave-packet.

Applying the Squeezing Transformation

Now that the time dependent harmonic oscillator system has been studied we will examine how to remove all quadratic terms from the Hamiltonian. Doing so will completely isolate the residual potential and allow for its effects on the wave-packet propagation to be studied. The quadratic terms can be removed by using a time dependent squeezing operation. This has been achieved in one dimension [8] and can be applied to this two dimensional system by treating the x and y direction independently.

The transformation of the wave-function will be performed in the $j = \{x, y\}$ direction by a squeezing operator $U_{sj}(t)$. The explicit form of $U_{sj}(t)$ will be derived later but for now we will assume, and later prove, that it will only act on functions and operators in the same j direction. This squeezing operator will transform the wave-function given in equation (14.45) as

$$\psi_{dprs}(x, y, t) = \hat{U}_{sy}^{-1}(t)\hat{U}_{sx}^{-1}(t)\psi_{dpr}(x, y, t). \quad (14.74)$$

This new wave-function can then be substituted into the Schrödinger equation (14.54) to give

$$\begin{aligned} i \frac{\partial \psi_{dprs}(x, y, t)}{\partial t} = & \left[\hat{U}_{sx}^{-1}(t) \left(\frac{\hat{p}_x^2}{2} + x^2 V'_{xx} \right) \hat{U}_{sx}(t) - i \hat{U}_{sx}^{-1}(t) \left(\frac{\partial \hat{U}_{sx}(t)}{\partial t} \right) \right. \\ & + U_{sy}^{-1}(t) \left(\frac{\hat{p}_y^2}{2} + y^2 V'_{yy} \right) \hat{U}_{sy}(t) - i \hat{U}_{sy}^{-1}(t) \left(\frac{\partial \hat{U}_{sy}(t)}{\partial t} \right) \\ & \left. + \hat{U}_{sy}^{-1}(t) \hat{U}_{sx}^{-1}(t) V_R(\hat{x}' + x_t, \hat{y}' + y_t) \hat{U}_{sy}(t) \hat{U}_{sx}(t) \right] \psi_{dprs}(x, y, t). \end{aligned} \quad (14.75)$$

Thus, we can directly see that the quadratic terms will be removed if the squeezing transformations obey the relations

$$i \hat{U}_{sx}^{-1}(t) \left(\frac{\partial \hat{U}_{sx}(t)}{\partial t} \right) = \hat{U}_{sx}^{-1}(t) \left(\frac{\hat{p}_x^2}{2} + x^2 V'_{xx} \right) \hat{U}_{sx}(t), \quad (14.76)$$

$$i \hat{U}_{sy}^{-1}(t) \left(\frac{\partial \hat{U}_{sy}(t)}{\partial t} \right) = \hat{U}_{sy}^{-1}(t) \left(\frac{\hat{p}_y^2}{2} + y^2 V'_{yy} \right) \hat{U}_{sy}(t). \quad (14.77)$$

Since each of these expressions are the same as in the one dimensional version of this calculation the same squeezing operator can be applied. The only difference is that the ladder operators a, a^\dagger and $\epsilon(t)$ will need to be substituted for the ones appropriate to the direction in which the squeezing is applied. Thus, for a complex parameter $\xi(t) = r(t)e^{i\chi(t)}$ the squeezing transformation in the j direction is [8]

$$\hat{U}_s(t) = \hat{S}(\xi_j(t)) \exp[i\hat{N}_j\Theta_j(t)], \quad (14.78)$$

where N_j is the number operator in the j direction, Θ_j a complex phase factor and $\hat{S}(\xi(t))$ is the squeezing operator [19]

$$\hat{S}(\xi_j(t)) = \exp \left[-\frac{\xi_j(t)}{2} \hat{a}_j^{\dagger 2} + \frac{\xi_j(t)}{2} \hat{a}_j^2 \right]. \quad (14.79)$$

The operators \hat{a}_j and \hat{a}_j^\dagger are the conventional ladder operators as opposed to the time dependent ones that have been discussed in the previous section. For this squeezing transformation to satisfy equations (14.76, 14.77) $\xi(t)$ will need to be specified. This is done by substituting the squeezing transformation (14.78) into the conditions (14.76, 14.77) and coefficients compared to specify $r_j(t)$, $\xi_j(t)$, $\Theta_j(t)$. The two sides of the equations can be compared by expressing the position and momentum operators in terms of \hat{a}_j , \hat{a}_j^\dagger and the $\epsilon_j(t)$ functions. This leads to conditions on $r_j(t)$, $\chi_j(t)$ and $\Theta_j(t)$ being [8]:

$$r_j(t) = \arctan \left(\frac{|\epsilon_j + \dot{\epsilon}_j|}{|\epsilon_j - \dot{\epsilon}_j|} \right), \quad (14.80)$$

$$e^{i\chi_j(t)} = -\frac{(\epsilon_j + \dot{\epsilon}_j) |\epsilon_j - \dot{\epsilon}_j|}{|\epsilon_j + \dot{\epsilon}_j| (\epsilon_j - \dot{\epsilon}_j)}, \quad (14.81)$$

$$e^{i\Theta_j(t)} = \frac{(\epsilon_j - \dot{\epsilon}_j)}{|\epsilon_j - \dot{\epsilon}_j|}, \quad (14.82)$$

where the time dependence of the ϵ_j functions has not been explicitly stated for convenience. The above relations can be substituted into the formula for the squeezing transformation (14.78) to eliminate the quadratic terms from the Hamiltonian (14.75). This will therefore, leave only a term containing the residual potential

$$i \frac{\partial \psi_{dprs}(x, y, t)}{\partial t} = \left[\hat{U}_{sy}^{-1}(t) \hat{U}_{sx}^{-1}(t) V_R(\hat{x}' + x_t, \hat{y}' + y_t) \hat{U}_{sy}(t) \hat{U}_{sx}(t) \right] \psi_{dprs}(x, y, t). \quad (14.83)$$

Since the residual potential depends on the operators \hat{x} and \hat{y} , transforming these is sufficient in order to specify the residual potential in the squeezed basis. These transformations are found by expressing \hat{x} and \hat{y} in terms of the ladder operators and using known results for the squeezing transformation acting upon the ladder operators [19]:

$$\hat{U}_{sx}^{-1}(t) \hat{x} \hat{U}_{sx}(t) = \text{Re}(\epsilon_x(t)) \hat{x} + \text{Im}(\epsilon_x(t)) \hat{p}_x, \quad (14.84)$$

$$\hat{U}_{sy}^{-1}(t) \hat{y} \hat{U}_{sy}(t) = \text{Re}(\epsilon_y(t)) \hat{y} + \text{Im}(\epsilon_y(t)) \hat{p}_y. \quad (14.85)$$

The residual potential depends on \hat{x}' and \hat{y}' as specified in equations (14.40, 14.41). Therefore, to apply the squeezing transformations to the residual potential we need to apply them to the rotated co-ordinates defined by (14.78) using the results from equations (14.84, 14.85):

$$\begin{aligned} \hat{x}'_s = \hat{U}_{sy}^{-1}(t) \hat{U}_{sx}^{-1}(t) \hat{x}' \hat{U}_{sy}(t) \hat{U}_{sx}(t) &= \cos(\theta(t)) [\text{Re}(\epsilon_x(t)) \hat{x} + \text{Im}(\epsilon_x(t)) \hat{p}_x] \\ &\quad + \sin(\theta(t)) [\text{Re}(\epsilon_y(t)) \hat{y} + \text{Im}(\epsilon_y(t)) \hat{p}_y], \end{aligned} \quad (14.86)$$

$$\begin{aligned} \hat{y}'_s = \hat{U}_{sy}^{-1}(t) \hat{U}_{sx}^{-1}(t) \hat{y}' \hat{U}_{sy}(t) \hat{U}_{sx}(t) &= \cos(\theta(t)) [\text{Re}(\epsilon_y(t)) \hat{y} + \text{Im}(\epsilon_y(t)) \hat{p}_y] \\ &\quad - \sin(\theta(t)) [\text{Re}(\epsilon_x(t)) \hat{x} + \text{Im}(\epsilon_x(t)) \hat{p}_x]. \end{aligned} \quad (14.87)$$

This transformation can be substituted into the Schrödinger equation (14.83) to isolate the evolution from the residual potential giving the main result of this analysis

$$i \frac{\partial \psi_{dprs}(x, y, t)}{\partial t} = V_R(\hat{x}'_s + x_t, \hat{y}'_s + y_t) \psi_{dprs}(x, y, t). \quad (14.88)$$

This equation gives the time evolution of a two dimensional wave-function that comes solely from the terms neglected by the Heller treatment. This will allow the time evolution of $\psi_{dprs}(x, y, t)$ to be computed and then transformed back into the original frame using the full series of transformations derived in this Chapter:

$$\psi(x, y, t) = \hat{D}_x(x_t, p_x) \hat{D}_y(y_t, p_y) e^{-i\phi_u(t)} \hat{U}_R(-\theta(t)) \hat{U}_{sx}(\xi_x(t)) \hat{U}_{sy}(\xi_y(t)) \psi_{dprs}(x, y, t). \quad (14.89)$$

14.4 Conclusions and Future Work

It has been shown how to perform a two-dimensional *extended* Gaussian wave-packet propagation. The equations for $\epsilon_x(t)$, $\epsilon_y(t)$ and $\theta(t)$ can be solved and then used to specify the transformation of the wave-function, and residual potential, alongside the Heller parameters. This amounts to adding additional differential equations to be solved numerically, which will allow for two dimensional propagation without the position space being discretised.

In the one dimensional extended Gaussian wave-packet approach the effects of the residual potential are computed by changing to a Fock basis and computing coefficients $a_n(t)$ of the $|n\rangle$ states. Similarly, the wave-function $\psi_{dprs}(x, y, t)$ can be put into a two dimensional Fock basis $|n_x, n_y\rangle$ with coefficients being computed in a similar way. In cases where the residual potential is orthogonal the results from Ref. [8] can be applied in each direction simultaneously.

Future work can be carried out to derive the coefficients using matrix elements of the residual potential where cross terms arise. Additionally, in future work the theory can be extended to a three dimensional propagation where there will be significant improvements in computation time compared with direct solving algorithms.

Acknowledgments

We acknowledge the support of the UK Defence Science and Technology Laboratory, grant No. DSTLX-1000138618.

14.5 Appendix A: Scaled Units in Numerical Simulations

In numerical simulations it is often useful to examine a system in scaled units as opposed to using specific values since this allows for the simulation to be applied to a variety of cases. Scaled units have been used throughout the paper to show the general trends of a system without worrying about the details of a specific physical system being studied.

In the quantum systems parameters will be made dimensionless through scalings often coming from the starting point of desiring the mass m and reduced Planck's constant \hbar to be unity. This is carried out by scaling the physical mass m' , position x' and time t' by:

$$m = \frac{m'}{m_s}, \quad x = \frac{x'}{x_s}, \quad t = \frac{t'}{t_s}, \quad (14.90)$$

with m_s , x_s and t_s being the scaling factors. A dimensionless mass $m = 1$ can be achieved simply by setting the mass scaling to be $m_s = m'$. Similarly a dimensionless time can be achieved by setting the time scaling $t_s = 1$ second. With the mass and time scaling chosen the length scale can be set such that $\hbar = 1$:

$$x_s = \sqrt{\frac{\hbar t_s}{m_s}}. \quad (14.91)$$

Thus, the complete set of scalings are

$$m_s = m', \quad x_s = \sqrt{\frac{\hbar}{m'}}, \quad t_s = 1 \text{ s}. \quad (14.92)$$

Using these conditions a quantum system can be simulated with dimensionless parameters and later be related to a physical system by using the inverse of the relations (14.90).

14.6 Appendix B: Action of the Angular Expectation Value

In order to examine the expectation value of the angular momentum operator we will examine its effect on a wave-packet that starts at rest. This result will apply to the wave function since we are examining a transformed Gaussian wave function that is in the centre of mass frame. The initial wave-function is defined by ($\hbar = 1$)

$$\psi(x, y, t) = \exp [i (\alpha_x x^2 + \alpha_y y^2 + \lambda xy + \gamma_t)]. \quad (14.93)$$

Comparing this wave-packet to the full Heller wave-packet ansatz (14.9) we can see that the initial position and momentum of $\psi(x, y, t)$ is zero.

The angular momentum operator is given by $\hat{L} = \hat{x}\hat{P}_y - \hat{y}\hat{P}_x$, so to calculate its expectation value we will first look at the effect of one of these terms. Acting on the wave-function given in equation (14.93) with the $\hat{x}\hat{P}_y$ term gives

$$\hat{P}_y \psi(x, y, t) = -i \frac{\partial \psi(x, y, t)}{\partial y} = (2\alpha_y y + \lambda x) \psi(x, y, t), \quad (14.94)$$

$$\hat{x}\hat{P}_y \psi(x, y, t) = (2\alpha_y xy + \lambda x^2) \psi(x, y, t). \quad (14.95)$$

The expectation value of this quantity can be found by integrating it with the mod square of the wave-function (14.93)

$$\begin{aligned} \langle \hat{x}\hat{P}_y \rangle &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (2\alpha_y xy + \lambda x^2) \\ &\times \exp [-2 (\text{Im}(\alpha_x)x^2 + \text{Im}(\alpha_y)y^2 + \text{Im}(\lambda)xy + \text{Im}(\gamma_t))] dx dy. \end{aligned} \quad (14.96)$$

This integral can be evaluated by splitting up the calculation into various parts, focusing on each part individually before bringing the parts back together to find the full solution. Firstly, the γ_t term in the above expression gives the normalisation of the wave-function.

This can be calculated relatively simply by integrating the mod square of the wavefunction defined by equation (14.93). The value of the normalisation is given by

$$\exp[-2\text{Im}(\gamma_t)] = \frac{1}{\pi} (4\text{Im}(\alpha_x)\text{Im}(\alpha_y) - \text{Im}(\lambda)^2)^{1/2}. \quad (14.97)$$

The first term (the xy term) in the integral (14.96) can be evaluated using exponential integral identities [20] to give the result

$$\begin{aligned} & 2\alpha_y \exp[-2\text{Im}(\gamma_t)] \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} xy \exp[-2(\text{Im}(\alpha_x)x^2 + \text{Im}(\alpha_y)y^2 + \text{Im}(\lambda)xy)] dx dy, \\ &= \frac{-\alpha_y \text{Im}(\lambda)}{4\text{Im}(\alpha_x)\text{Im}(\alpha_y) - \text{Im}(\lambda)^2}, \end{aligned} \quad (14.98)$$

where the normalisation from (14.97) has been used. Similarly the second term in (14.96) can also be evaluated

$$\begin{aligned} & \lambda \exp[-2\text{Im}(\gamma_t)] \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x^2 \exp[-2(\text{Im}(\alpha_x)x^2 + \text{Im}(\alpha_y)y^2 + \text{Im}(\lambda)xy)] dx dy, \\ &= \frac{\lambda \text{Im}(\alpha_y)}{4\text{Im}(\alpha_x)\text{Im}(\alpha_y) - \text{Im}(\lambda)^2}. \end{aligned} \quad (14.99)$$

Thus, by putting together the two expressions (14.98, 14.99) the expectation value of $\hat{x}\hat{P}_y$ can be found by splitting up λ and α_y into their real and imaginary components

$$\langle \hat{x}\hat{P}_y \rangle = \frac{\lambda \text{Im}(\alpha_y) - \alpha_y \text{Im}(\lambda)}{4\text{Im}(\alpha_x)\text{Im}(\alpha_y) - \text{Im}(\lambda)^2} = \frac{\text{Re}(\lambda)\text{Im}(\alpha_y) - \text{Re}(\alpha_y)\text{Im}(\lambda)}{4\text{Im}(\alpha_x)\text{Im}(\alpha_y) - \text{Im}(\lambda)^2}. \quad (14.100)$$

A similar result can be obtained by going through the same process for the other half of the angular momentum operator i.e. calculating the expectation value of $\langle \hat{y}\hat{P}_x \rangle$. The result of such a calculation is

$$\langle \hat{y}\hat{P}_x \rangle = \frac{-\text{Re}(\lambda)\text{Im}(\alpha_x) + \text{Re}(\alpha_x)\text{Im}(\lambda)}{4\text{Im}(\alpha_x)\text{Im}(\alpha_y) - \text{Im}(\lambda)^2}. \quad (14.101)$$

Thus, the expectation value of the full angular momentum operator can be found by taking the difference of equations (14.100) and (14.101)

$$\langle L \rangle = \langle \hat{x}\hat{P}_y \rangle - \langle \hat{y}\hat{P}_x \rangle = \frac{\text{Re}(\Delta\alpha)\text{Im}(\lambda) - \text{Re}(\lambda)\text{Im}(\Delta\alpha)}{4\text{Im}(\alpha_x)\text{Im}(\alpha_y) - \text{Im}(\lambda)^2}, \quad (14.102)$$

where $\Delta\alpha = \alpha_x - \alpha_y$. The above expression gives the full time evolution of the expectation value of angular momentum as long as the solutions for α_x , α_y and λ are known.

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Cite this work as:

G. Wilson and B. M. Garraway, Propagation of Non-Gaussian Wave-Packets in Two Dimensions, in A. Dodonov and C. C. H. Ribeiro (Eds.), Proceedings of the Second International Workshop on Quantum Nonstationary Systems, pp. 227–248 (LF Editorial, São Paulo, 2024). ISBN: 978-65-5563-446-4.

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