EVOLUTION OF WAVE PACKETS UNDER SEMICLASSICAL APPROXIMATIONS

An Undergraduate Research Scholars Thesis

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This project did not require approval from the Texas A&M University Research Compliance & Biosafety office.

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ABSTRACT

Evolution of Wave Packets Under Semiclassical Approximations

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In quantum mechanics, the propagator specifies the probability amplitude for a particle to travel from one position in space to another in a given period of time. Utilizing a propagator, as well as a basic Gaussian wave packet, one can integrate the two quantities against one another to construct a full quantum wave function — a function that describes the behavior of a quantum particle. Using previously computed propagators, we present a visual representation of this semi-classical wave packet behavior for a particle interacting with a 'ceiling' boundary. We explain the roles of the parameters embedded in the Gaussian wave packets and examine their effects on the resulting wave function. Two different types of propagator expressions have been derived, one in terms of initial position data and another in terms of initial momentum data. We present results computed by both methods and elaborate upon the regimes in which one particular method is preferred. Additionally, we present the software developed to conduct this research and detail how it is used such that it may be adapted for future use.

DEDICATION

To my friends at Texas A&M.

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Contributors

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1. INTRODUCTION AND PREVIOUS WORK

1.1 Quantum Dynamics

1.1.1 The Quantum Wave Function

The wave function of quantum mechanics, denoted as Ψ, is the mathematical representation of the state of a quantum system. In contrast to the deterministic nature of classical mechanics, the wave function of quantum mechanics is a complex-valued probability amplitude such that the probability of a possible measurement made on the system may be derived from it. The wave function is governed by the time-dependent Schrödinger equation (TDSE).

$$i\hbar\frac{\partial\Psi(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{x},t) + V(\mathbf{x})\Psi(\mathbf{x},t) \tag{1.1}$$

Here, $\mathbf{x}$ denotes the position vector in $\mathbb{R}^3$. Solutions of the TDSE are expressed as plane waves propagating through both real and complex space. For a free particle ($V(\mathbf{x}) = 0$), the wave function takes the following form

$$\Psi(\mathbf{x},t) = Ae^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)} \tag{1.2}$$

with wave vector $\mathbf{k}$, frequency ω, and amplitude A.

1.1.2 The Propagator

The TDSE may alternatively be solved via its Green's Function. The Green's Function of the TDSE is the referred to as the *propagator*. The propagator, denoted as $U(\mathbf{x},\mathbf{y},t)$, describes the evolution of the wave function in time as the particle propagates from the state at initial position $\mathbf{y}$ to the state at final position $\mathbf{x}$. When integrated against the initial wave function of the system, the overall result yields the time-evolved wave function.

$$\Psi(\mathbf{x},t) = \int U(\mathbf{x},\mathbf{y},t)\Psi(\mathbf{y},0)d\mathbf{y} \tag{1.3}$$

One may also express $\Psi(\mathbf{x}, t)$ in terms of initial momentum data via a Fourier transform of Equation 1.3 where factors of 2π have been suppressed and $\hbar$ is set equal to 1.

$$\Psi(\mathbf{x}, t) = \int U(\mathbf{x}, \mathbf{p}, t)\Phi(\mathbf{p}, 0)d\mathbf{p} \tag{1.4}$$

Note that in Equation 1.3 the propagator is integrated against $\Psi(\mathbf{x}, 0)$ - the wave function in the position representation, yet in Equation 1.4 the propagator is integrated against $\Phi(\mathbf{p}, 0)$ - the wave function in the momentum representation. The propagator allows one to determine the wave function of the system for either initial position data, or initial momentum data depending upon the available information of the physical scenario one wishes to study. For this research, we will adopt a new sign convention for $\bar{p}$ than that of [1], and take these initial wave functions as

$$\Psi(\mathbf{y}, 0) = \left(\frac{2}{\pi\gamma}\right)^{1/4} e^{i\bar{p}y - i\frac{(y-\bar{y})^2}{\gamma}} \tag{1.5}$$

$$\Phi(\mathbf{p}, 0) = \left(\frac{\gamma}{2\pi}\right)^{1/4} e^{-i(p-\bar{p})\bar{y} - i\gamma\frac{(p-\bar{p})^2}{4}} \tag{1.6}$$

The parameter $\bar{y}$ corresponds to the average initial position of the particle. $\bar{p}$ corresponds to the average initial momentum of the particle. γ prescribes the width of the wavepacket in position space. Via a Fourier transform, the width in momentum space becomes $4/\gamma$. In this work, we choose $\gamma = 2$ such that the widths are equivalent in both representations. The Fourier transform conventions utilized in this work are detailed in [2] and are

$$\phi(\mathbf{p}) = \frac{1}{\sqrt{2\pi}} \int d\mathbf{x}\psi(\mathbf{x})e^{-i\mathbf{p}\cdot\mathbf{x}} \tag{1.7}$$

$$\psi(\mathbf{y}) = \frac{1}{\sqrt{2\pi}} \int d\mathbf{p}\phi(\mathbf{p})e^{+i\mathbf{p}\cdot\mathbf{x}} \tag{1.8}$$

1.2 The WKB Approximation

1.2.1 Classical Theory

In semiclassical theory, we seek to understand the evolution of the quantum wave function of a particle traversing a classical path. Solutions of the classical theory are path functions **q** with

$$\mathbf{q}(0) = \mathbf{y} \qquad\qquad \mathbf{q}(t) = \mathbf{x} \tag{1.9}$$

For a given **x**, **y**, and t there may be a single path, no path, or several paths. In constructing the propagator for a particle we will sum over all available paths. Similarly, these conditions may be re-expressed in terms of the initial momentum as

$$m\dot{\mathbf{q}}(0) = \mathbf{p} \qquad\qquad \mathbf{q}(t) = \mathbf{x} \tag{1.10}$$

where ‘dot’ denotes a derivative in time. In classical theory, the *Lagrangian* L of the system characterizes the dynamics of the system. The Lagrangian is defined as

$$L = T - V \tag{1.11}$$

where T and V denote the kinetic and potential energy respectively. For our classical system, we write the Lagrangian as

$$L = \frac{m}{2}\dot{\mathbf{q}}^2 - V(\mathbf{q}) \tag{1.12}$$

To obtain the equations of motion governing a dynamical system, we use the *action* S, which is related to the Lagrangian by

$$S = \int dt\, L(\mathbf{q}, \dot{\mathbf{q}}, t) \tag{1.13}$$

Classically, the action is a fundamental quantity used in deriving the Euler-Lagrange equations of motion via the *Principle of Least Action*. In the semiclassical approximation, we will utilize the action to aid in the construction of the propagator as detailed in the following subsection.

1.2.2 The WKB Ansatz

The semiclassical, or WKB, ansatz approximates the quantum solution by a sum over all classical paths from the initial point to the final point. This theory is developed in many references, such as [3], [4], [5]. The contribution of each classical path to U takes the form

$$U(\mathbf{x}, t) = A(\mathbf{x}, t)e^{iS(\mathbf{x},t)/\hbar} \tag{1.14}$$

1.3 Linear Potential

In this thesis, we wish to study a 1-dimensional system with an impenetrable barrier at the origin and a linear potential. The potential of this system is

$$V(\mathbf{q}) = -\alpha\mathbf{q} \tag{1.15}$$

where **q** represents the position of the particle, and α characterizes the strength of the potential. For positive values of α, the barrier acts as a 'ceiling' and the particle may bounce off at most once. If α is negative, the barrier will act as a 'floor' and will have, in principle, an infinite number of bounces. This work is a continuation of [1] in which only the ceiling case is considered for two different types of initial data: initial position **y** or initial momentum **p**.

1.4 Classification of Paths

Note that henceforth all work will be done in one spatial dimension and thus the position vectors **x**, **y** and momentum vector **p** will now be referred to by x, y and p.

1.4.1 Free Particle

The particle in the absence of a potential, or free particle, is a very good test of the theory as it greatly reduces the difficulty of evaluating the total wave function. The momentum space propagator of the free particle is derived in [6]. The propagator is (using $m = 1/2$ and $\hbar = 1$)

$$U_{Free}(x, p, t) = \frac{1}{\sqrt{2\pi}}\exp\Big[ip(x - pt)\Big] \tag{1.16}$$

Via the Fourier transform defined in Equation 1.8, the position space propagator is

$$U_{Free}(x,y,t) = \frac{1}{\sqrt{4i\pi t}}\text{exp}\Big[\frac{i(x-y)^2}{4t}\Big] \tag{1.17}$$

1.4.2 Direct Paths

In reference [1], the direct paths are classified into three separate categories:

- Type (i) - Rightward path.
- Type (ii) - Leftward path.
- Type (iii) - Turning path.

The direct path propagators, equations (109a) and (109b) of [1], are restated here for convenience. Note, there appears to be a typo in [1] equation (109a); in this thesis we will construct the propagator using the correct action from equation (103a). The direct propagators are

$$U_{Direct}(x,p,t) = \frac{1}{\sqrt{4i\pi t}}\text{exp}\Big[i\Big(\frac{2t^3}{3} + t^2\Big(\frac{x-y}{t} - t\Big) + t\Big(\frac{1}{4}\Big(\frac{x-y}{t} - t\Big)^2 + y\Big)\Big)\Big] \tag{1.18}$$

$$U_{Direct}(x,y,t) = \frac{1}{\sqrt{2\pi}}\text{exp}\Big[-\frac{i}{3}(3p^2t + t^3 + 3p(t^2 - x) - 3tx)\Big] \tag{1.19}$$

1.4.3 Bounce Paths

The remaining possible paths to consider are the paths in which the particle interacts directly with the ceiling and changes direction. We will aptly refer to trajectories of this type as bounce paths. The bounce propagators are

$$\begin{aligned} U_{Bounce}(x,p,t) = &\frac{-1}{\sqrt{2\pi}}\sqrt{\frac{p+b_p}{\sqrt{(p+t)+3x}}} \\ &\times \text{exp}\Big[i\Big(\frac{-1}{3}\Big[b_p^3 + (t-b_p)^3\Big] - pb_p(3p+2b_p)\Big)\Big] \\ &\times \text{exp}\Big[i\Big((t-b_p)(x+(p+b_p)^2)\Big)\Big] \end{aligned} \tag{1.20}$$

$$
\begin{aligned}
U_{Bounce}(x,y,t) = \frac{1}{\sqrt{4\pi i}}&\sqrt{\frac{y-b_y^2}{-3tb_y^2+2(t^2-x-y)b_y+3yt}} \\
&\times \exp\Big[i\Big(\frac{2}{3}b_y^3 - b_y^2\Big[\frac{y}{t}+b_y\Big] + b_y\Big(\frac{1}{4}\Big[\frac{y}{t}+b_y\Big]^2+y\Big)\Big)\Big] \\
&\times \exp\Big[i\Big(\frac{2}{3}(t-b_y)^3 + (t-b_y)^2\Big[\frac{x}{t}-(t-b_y)\Big]\Big)\Big] \\
&\times \exp\Big[i\frac{(t-b_y)}{4}\Big(\frac{x}{t}-(t-b_y)\Big)^2\Big]
\end{aligned} \tag{1.21}
$$

Here b_p and b_y have been introduced. These quantities refer to the time in which the bounce occurs and thus have units of $[t]$. The solutions of b_p and b_y are discussed in great detail in [1], and are restated below.

$$
b_p = \frac{1}{3}\Big(2t - p - \sqrt{(p+t)^2+3x}\Big) \tag{1.22}
$$

$$
b_y = \frac{t}{2} + \sqrt{\frac{t^2+2(x+y)}{3}}sin\Big[\frac{1}{3}sin^{-1}\frac{3\sqrt{3}t(y-x)}{(t^2+2(x+y))^{3/2}}\Big] \tag{1.23}
$$

1.4.4 Addition of Paths

The constraints on initial momentum given (x,t) are shown below. Both the turning paths and bounce paths are divided into two subcategories: Type (iiia), Type (iiib) and Bounce (a), Bounce (b). These distinctions arise from differences in domain in position and momentum space. The divide occurs at $x = t^2$ and is discussed further in [1]. These domains are utilized as the domain of integration in calculating the wave function for each trajectory. The domains are given in the following tables.

Table 1.1: Trajectory domains in momentum space. Endpoints not included.

Path Type	$x \in$	$p \in$
Type (i)	(t^2, ∞)	$(0, \frac{x-t^2}{2t})$
Type (ii)	$(0, \infty)$	$(-\infty, -t)$
Type (iiia)	$(0, t^2)$	$(-t, \sqrt{x} - t)$
Type (iiib)	(t^2, ∞)	$(-t, 0)$
Bounce (a)	$(0, t^2)$	$(-\infty, \sqrt{x} - t)$
Bounce (b)	(t^2, ∞)	$(-\infty, \frac{x-t^2}{2t})$

Table 1.2: Trajectory domains in position space. Endpoints not included.

Path Type	$x \in$	$y \in$
Type (i)	(t^2, ∞)	$(0, x - t^2)$
Type (ii)	$(0, \infty)$	$(x + t^2, \infty)$
Type (iiia)	$(0, t^2)$	$((\sqrt{x} - t^2)^2, x + t^2)$
Type (iiib)	(t^2, ∞)	$(x - t^2, x + t^2)$
Bounce (a)	$(0, t^2)$	$((\sqrt{x} - t^2)^2, \infty)$
Bounce (b)	(t^2, ∞)	$(0, \infty)$

As mentioned, all trajectories may be divided into paths valid for $x < t^2$ and $x > t^2$. For $x < t^2$, the interval of integration for the direct paths over p is

$$\begin{aligned}(-\infty, \sqrt{x} - t) &= (-\infty, -t) \cup (-t, \sqrt{x} - t)\\ &= \text{Type (ii)} \cup \text{Type (iiia)}\end{aligned}$$

For $x < t^2$, the interval of integration for the direct paths over y is

$$\begin{aligned}((\sqrt{x}-t)^2,\infty) &= ((\sqrt{x}-t)^2, x+t^2) \cup (x+t^2,\infty)\\ &= \text{Type (iiia)} \cup \text{Type (ii)}\end{aligned}$$

For $x > t^2$, the interval of integration for the direct paths over p is

$$\begin{aligned}(-\infty,\frac{x-t^2}{2t}) &= (-\infty,-t) \cup (-t,0) \cup (0,\frac{x-t^2}{2t})\\ &= \text{Type (ii)} \cup \text{Type (iiib)} \cup \text{Type (i)}\end{aligned}$$

For $x > t^2$, the interval of integration for the direct paths over y is

$$\begin{aligned}(0,\infty) &= (0,x-t^2) \cup (x-t^2,x+t^2) \cup (x+t^2,\infty)\\ &= \text{Type (i)} \cup \text{Type (iiib)} \cup \text{Type (ii)}\end{aligned}$$

Thus it has been demonstrated that the domain of integration for $x < t^2$ and $x > t^2$ correspond to the same paths in both momentum and position space and should lead to the same wave function contribution. To include the bounce contribution we simply add Bounce (a) to the $x < t^2$ paths and Bounce (b) to the $x > t^2$ paths. The contribution of the direct and bounce paths yield the complete wave function for the particle and results for this wave function are presented in Section 3.

1.5 Classical Solutions

In the limit $\hbar \to 0$ we expect to recover the classical picture. However in the semiclassical picture, the classical results are still of use. Classically, the dynamics of the particle are described by

$$q(t) = t^2 + 2\bar{p}t + \bar{y} \tag{1.24}$$

In the quantum picture, this position q corresponds to the centroid of the wave packet. As the ceiling boundary is placed at the origin, the paths in which the particle bounces off of the ceiling will take on a new trajectory after the bounce. The time of the bounce can be calculated by setting

Equation 1.24 equal to zero. The time of bounce, b, is

$$b = -\bar{p} - \sqrt{\bar{p}^2 - \bar{y}} \tag{1.25}$$

After the bounce occurs, the particle follows a new trajectory q', and the previous trajectory q should be replaced by the following.

$$q' = (t - b)^2 + 2(t - b)\sqrt{\bar{p}^2 - \bar{y}} \tag{1.26}$$

1.6 Boundary Conditions

There are two different boundary conditions that may be selected when analyzing the wave function at the ceiling ($x = 0$). The *Dirichlet* boundary condition states that the complete wave function must vanish at the origin.

$$\Psi(0, t) = 0 \tag{1.27}$$

The correct WKB approximation for the Dirichlet boundary condition is the difference between the direct and bounce contributions, $U_{Direct} - U_{Bounce}$. The alternative to the Dirichlet boundary is the *Neumann* boundary condition which states that the spatial derivative of the wave function must vanish at the origin.

$$\frac{\partial \Psi(0, t)}{\partial x} = 0 \tag{1.28}$$

The correct WKB approximation for the Neumann boundary condition is the sum between the direct and bounce contributions, $U_{Direct} + U_{Bounce}$.

In Section 3 we display wave function results following the Neumann boundary condition.

2. METHODS

We wish to study how the variables $\bar{y}$, $\bar{p}$, and t affect the accuracy of the approximation in position space and momentum space. To better understand these effects on the overall wave function, we will utilize Wolfram Mathematica to compute and plot the cumbersome integrals outlined in Equations 1.3 and 1.4. Two files are attached in Appendices A and B. Appendix A contains the TotalWaveFunction.nb file which is used to compute all direct and bounce path contributions to the wave function. Appendix B contains the FreeWaveFunction.nb file which is presented as an example of how the approximation scheme would ideally function. The free particle approximation is identical in both the position and momentum representations and thus should be used as a reference when studying the results of the more complicated paths computed in Appendix A.

Note that in Mathematica, text written in the form (*Comment*) is a comment and is not computed by the program.

2.1 Structure of TotalWaveFunction.nb

2.1.1 Declaration of Formulae

Variables $\bar{y}$, $\bar{p}$, and t are declared globally prior to any computation. Relevant quantities including initial Gaussian wave packets and propagators for both direct and bounce paths are defined. The naming conventions chosen for the functions defined in the Mathematica program and the quantities the represent from Section 1 are detailed in Table 2.1. In the file, the corresponding equation number from Section 1 is presented as a comment following the definition of the function.

Table 2.1: Declaration of Wave Packets and Propagators.

Mathematica Function	**Corresponding Symbol From Section I**
`YBAR`	$\bar{y}$
`PBAR`	$\bar{p}$
`TIME`	t
`psi[y_]`	$\Psi(\mathbf{y}, 0)$
`phi[p_]`	$\Phi(\mathbf{p}, 0)$
`Ud[y_]`	$U_{Direct}(x, y, t)$
`ud[p_]`	$U_{Direct}(x, p, t)$
`by`	b_y
`bp`	b_p
`Ub[y_]`	$U_{Bounce}(x, y, t)$
`ub[p_]`	$U_{Bounce}(x, p, t)$
`PSIY`	$\Psi(\mathbf{x}, t)$
`PSIP`	$\Psi(\mathbf{x}, t)$

2.1.2 Computation of Wave Function

To compute the overall wave function the integrals must be split into a sum of several simple integrals that the program is more apt to handle.

For the direct path contributions, the integral is computed with $\bar{y}$, $\bar{p}$, and t left as undefined variables. Prior to the evaluation of each integral, the domain of integration in both position and momentum space is restated from Tables 1.1 and 1.2 for convenience. The naming of the functions relating to the direct path computations is detailed in Table 2.2.

For the bounce path contributions, the values of $\bar{y}$, $\bar{p}$, and t must be defined in the integrand prior to integration. Alternatively, the bounce path contributions must also be computed using numerical integration via Mathematica's `NIntegrate` command due to the highly oscillatory nature of the integrals. The naming of the functions relating to the bounce path computations is detailed in Table 2.3.

Table 2.2: Computation of Direct Path Types.

Mathematica Function	**Interpretation of Function**
`type1y`	Contribution to wave packet due to Type (i) paths in position space
`type1p`	Contribution to wave packet due to Type (i) paths in momentum space
`type2y`	Contribution to wave packet due to Type (ii) paths in position space
`type2p`	Contribution to wave packet due to Type (ii) paths in momentum space
`type3ay`	Contribution to wave packet due to Type (iiia) paths in position space
`type3ap`	Contribution to wave packet due to Type (iiia) paths in momentum space
`type3by`	Contribution to wave packet due to Type (iiib) paths in position space
`type3bp`	Contribution to wave packet due to Type (iiib) paths in momentum space

Table 2.3: Computation of Bounce Path Types.

Mathematica Function	**Interpretation of Function**
`tbounce`	Fixes value of t for all bounce related quantities
`psifixed[y_]`	Fixes value of $\bar{y}$, $\bar{p}$, t for `psi[y_]` prior to integration
`phifixed[p_]`	Fixes value of $\bar{y}$, $\bar{p}$, t for `phi[p_]` prior to integration
`bounceay`	Contribution to wave packet due to Bounce (a) paths in position space
`bounceap`	Contribution to wave packet due to Bounce (a) paths in momentum space
`bounceby`	Contribution to wave packet due to Bounce (b) paths in position space
`bouncebp`	Contribution to wave packet due to Bounce (b) paths in momentum space

2.1.3 Plot of Complete Wave Function

The results of the integration are plotted. The direct paths are summed as prescribed in Section 1.4.4. and the corresponding bounce paths are added as mentioned in Section 1.6. Note that regardless of integration over y or p, both plots are of $\Psi(\mathbf{x}, t)$ and thus calculations via both methods are ideally expected to resemble one another. The naming of the functions relating to the presentation of the total wave function is detailed in Table 2.4.

Table 2.4: Presentation of Complete Wave Function.

Mathematica Function	**Interpretation of Function**
`direct1y`	Addition of direct path contributions for $x < t^2$ in position space
`direct1p`	Addition of direct path contributions for $x < t^2$ in momentum space
`direct2y`	Addition of direct path contributions for $x > t^2$ in position space
`direct2p`	Addition of direct path contributions for $x > t^2$ in momentum space
`final1y`	All contributions for $x < t^2$ in position space
`final1p`	All contributions for $x < t^2$ in momentum space
`final2y`	All contributions for $x > t^2$ in position space
`final2p`	All contributions for $x > t^2$ in momentum space
`PSIY`	$\Psi(\mathbf{x}, t)$
`PSIP`	$\Psi(\mathbf{x}, t)$

2.2 Structure of Free.nb

2.2.1 Declaration of Formulae

Relevant quantities including initial Gaussian wave packets and propagators for both direct and bounce paths are defined. The naming conventions chosen for the functions defined in the Mathematica program and the quantities they represent from Section 1 are detailed in Table 2.5. In the file, the corresponding equation number from Section 1 is presented as a comment following the definition of the function.

Table 2.5: Declaration of Free Wave packets and Propagators.

Mathematica Function	**Corresponding Symbol From Section 1**
`psi[y_]`	$\Psi(\mathbf{y}, 0)$
`phi[p_]`	$\Phi(\mathbf{p}, 0)$
`Uf[y_]`	$U_{Free}(x, y, t)$
`uf[p_]`	$U_{Free}(x, p, t)$

2.2.2 *Computation of Wave Function*

Similar to the direct paths, the integrals may be handled by Mathematica without need for defining $\bar{y}$, $\bar{p}$, t prior to integration. The naming of the functions relating to the bounce path computations is detailed in Table 2.6.

Table 2.6: Computation of Free Particle Wave Function.

Mathematica Function	**Interpretation of Function**
`freey`	Wave function calculated in position space
`freep`	Wave function calculated in momentum space
`test`	Demonstrates that `freey` and `freep` are equal
`free[x_, t_, g_, yb_, pb_]`	Renaming of `freey` and `freep` into a single function

2.2.3 *Plot of Complete Wave Function*

Because the wave function is the same for each method of computation, Mathematica's `Manipulate` command is used to vary $\bar{y}$, $\bar{p}$, t. This eliminates the need to run the full program each separate time these variables are changed. The naming of the functions relating to the presentation of the total wave function is detailed in Table 2.7.

Table 2.7: Presentation of Free Particle Wave Function.

Mathematica Function	**Interpretation of Function**
`PSI`	$\Psi(\mathbf{x}, t)$
`PSIDynamic`	$\Psi(\mathbf{x}, t)$ with animation

3. RESULTS

The wave function results for various values of $\bar{y}$ and $\bar{p}$ are presented. Values of $\bar{y}$ must be positive and should also be larger than the wave packet width. Select values of $\bar{y}$ have been chosen to be $20, 15, 10, 5$. Values of $\bar{p}$ may be chosen to be negative or positive. Negative values of $\bar{p}$ are necessary for a bounce, but not sufficient. Select values of $\bar{p}$ have been chosen to be $5, 0, -5, -10, -15$. For each pair of $\bar{y}$, $\bar{p}$ the first line of plots correspond to the y-space calculation and the second line of plots correspond to the p-space calculation. The three plots are to be read from left to right with time increasing chronologically. Select values of t have been chosen to be $1, 2, 3$. Prior to the presentation of each wave function a table is presented to display the expected centroid of the wave packet. This position, q, as well as the time of bounce, b, are calculated for the specific values of $\bar{y}$, $\bar{p}$ using Equations 1.24, 1.25, 1.26. All plots have domain $0 \leq x \leq 50$ for consistency in comparing wave functions.

3.1 $\bar{\mathbf{y}} = \mathbf{20}$

Table 3.1: Expected position of particle with $\bar{y} = 20$.

$\bar{p}$	b	$t = 1$	$t = 2$	$t = 3$
5	N/A	$q = 31$	$q = 44$	$q = 59$
0	N/A	$q = 21$	$q = 24$	$q = 29$
-5	2.76	$q = 11$	$q = 4$	$q = 1.11$
-10	1.06	$q = 1$	$q = 17.78$	$q = 38.56$
-15	0.68	$q = 9.20$	$q = 39.47$	$q = 71.74$

```
(* yb=20 pb=5 *)
```

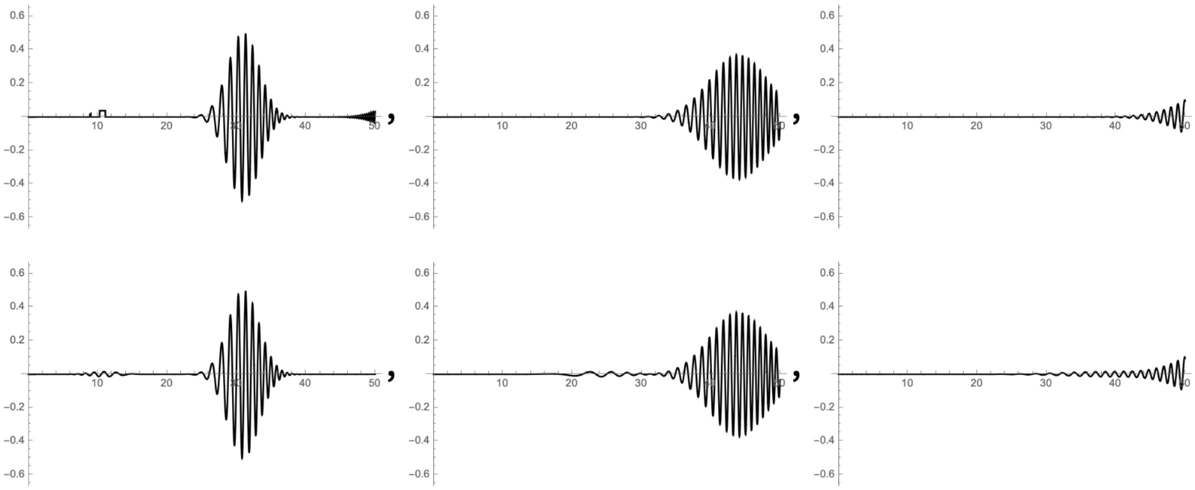


Figure 3.1: $\bar{y} = 20$, $\bar{p} = 5$.

```
(* yb=20 pb=0 *)
```

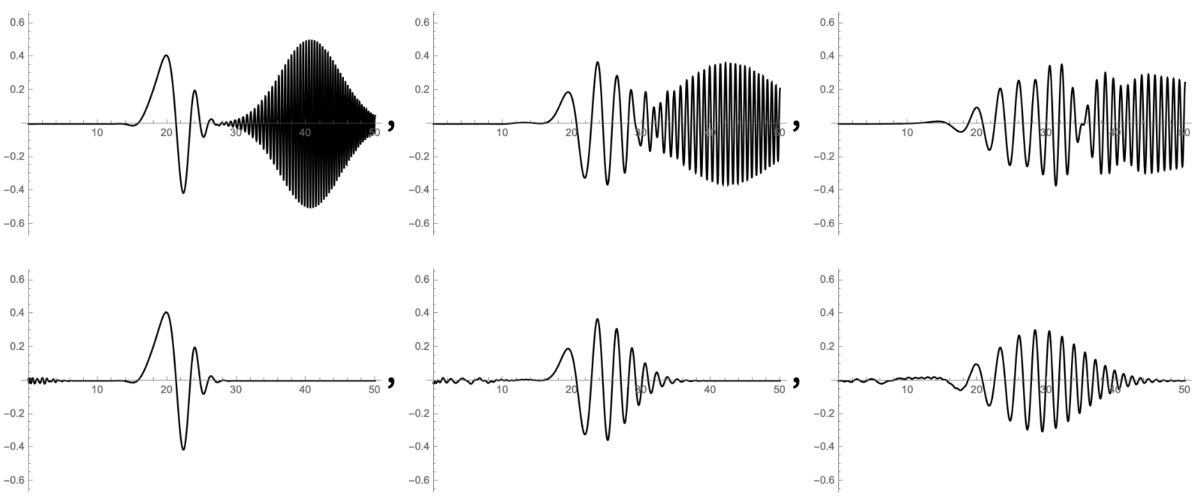


Figure 3.2: $\bar{y} = 20$, $\bar{p} = 0$.

```
(* yb=20 pb=-5 *)
```

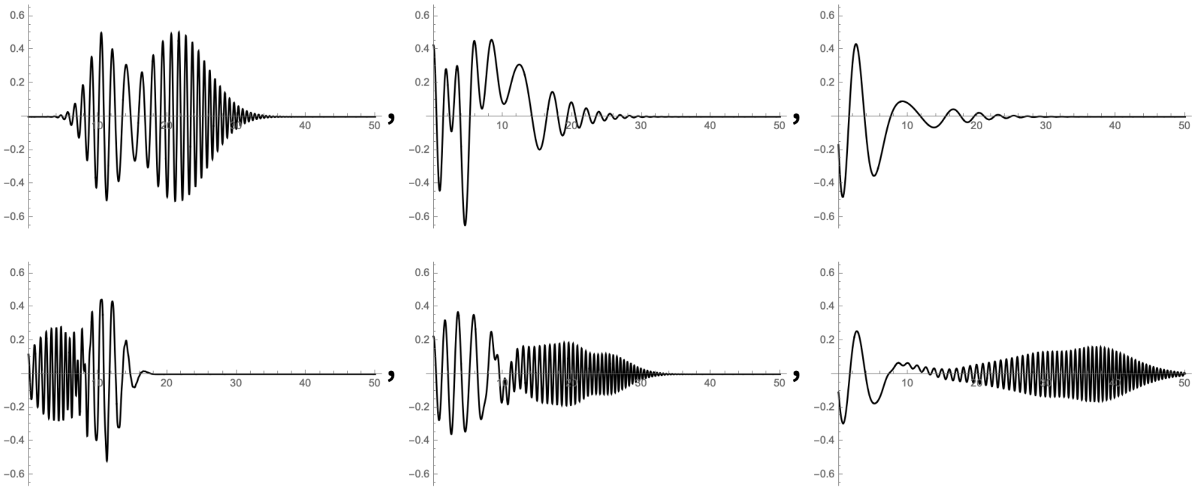


Figure 3.3: $\bar{y} = 20$, $\bar{p} = -5$.

```
(* yb=20 pb=-10 *)
```

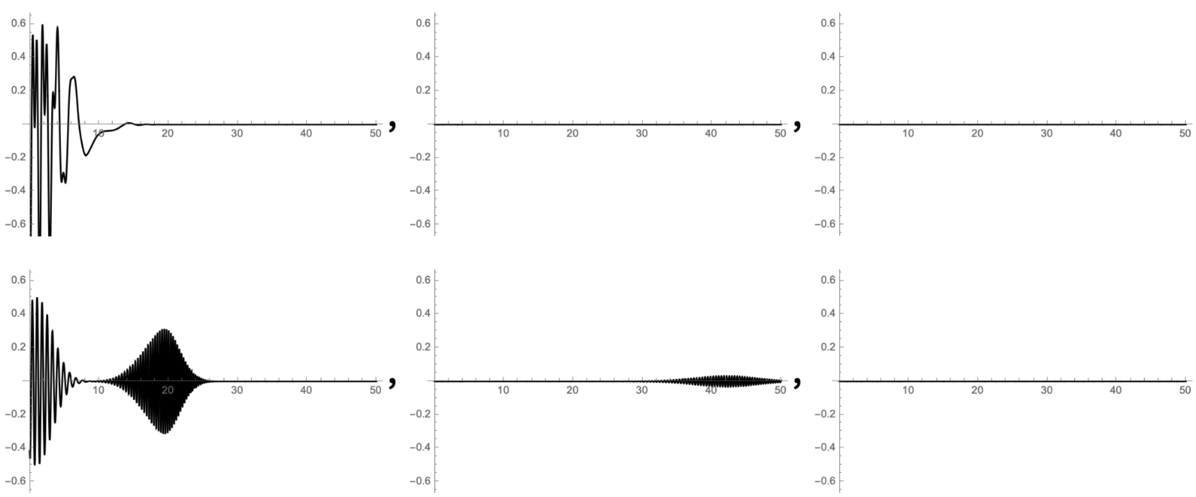


Figure 3.4: $\bar{y} = 20$, $\bar{p} = -10$.

```
(* yb=20 pb=-15 *)
```

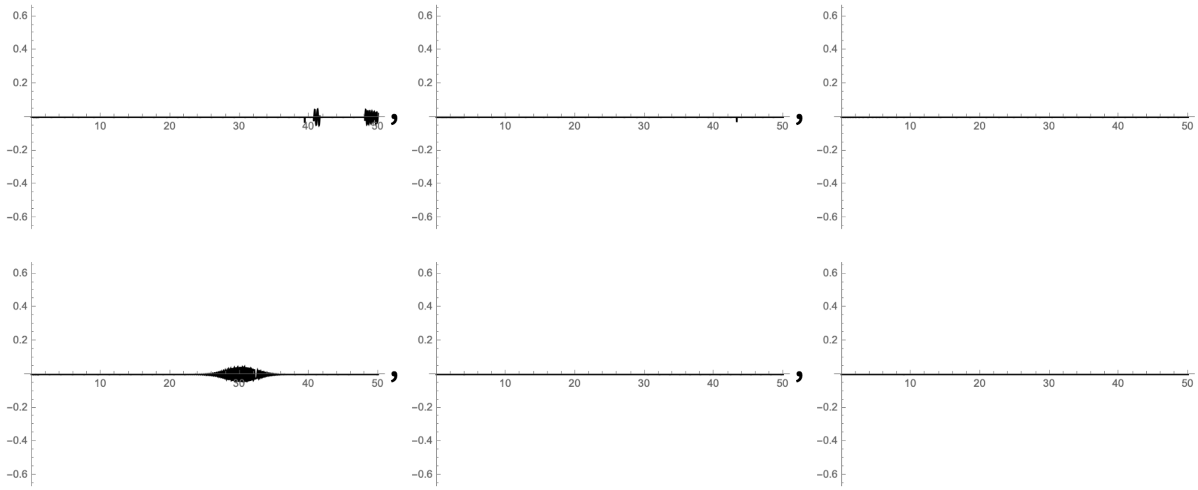


Figure 3.5: $\bar{y} = 20$, $\bar{p} = -15$.

3.2 $\bar{\mathbf{y}} = \mathbf{15}$

Table 3.2: Expected position of particle with $\bar{y} = 15$.

$\bar{p}$	b	$t = 1$	$t = 2$	$t = 3$
5	N/A	$q = 26$	$q = 39$	$q = 54$
0	N/A	$q = 16$	$q = 19$	$q = 24$
-5	1.83	$q = 6$	$q = 1.05$	$q = 8.70$
-10	0.78	$q = 4.10$	$q = 23.97$	$q = 45.85$
-15	0.50	$q = 14.48$	$q = 45.45$	$q = 78.41$

```
(* yb=15 pb=5 *)
```

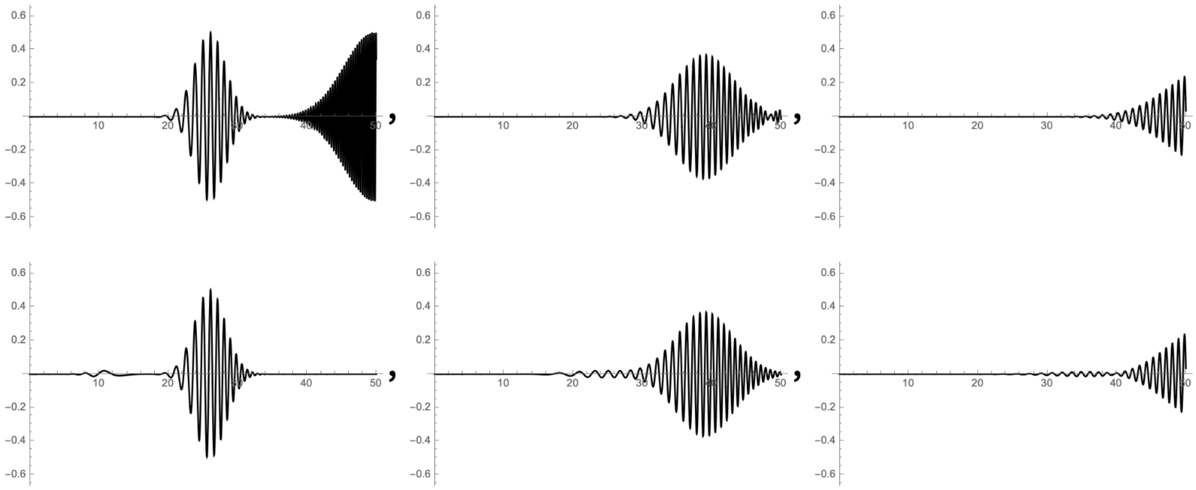


Figure 3.6: $\bar{y} = 15$, $\bar{p} = 5$.

```
(* yb=15 pb=0 *)
```

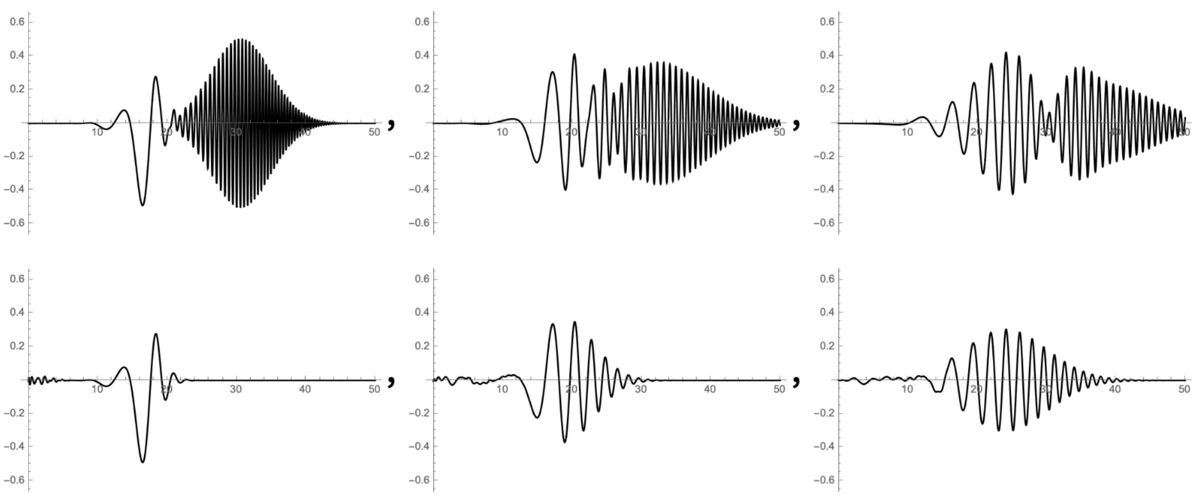


Figure 3.7: $\bar{y} = 15$, $\bar{p} = 0$.

```
(* yb=15 pb=-5 *)
```

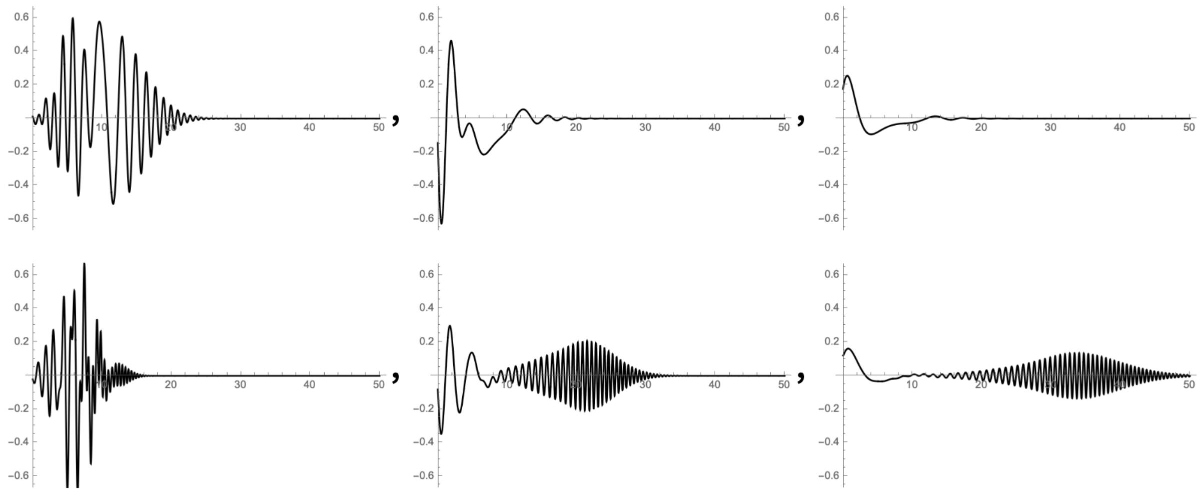


Figure 3.8: $\bar{y} = 15, \bar{p} = -5$.

```
(* yb=15 pb=-10 *)
```

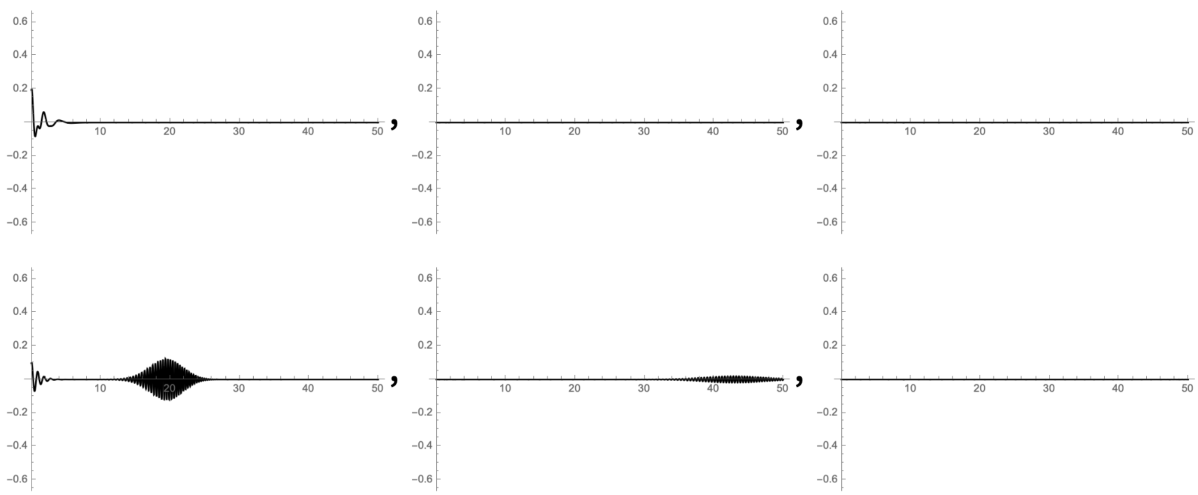


Figure 3.9: $\bar{y} = 15, \bar{p} = -10$.

```
(* yb=15 pb=-15 *)
```

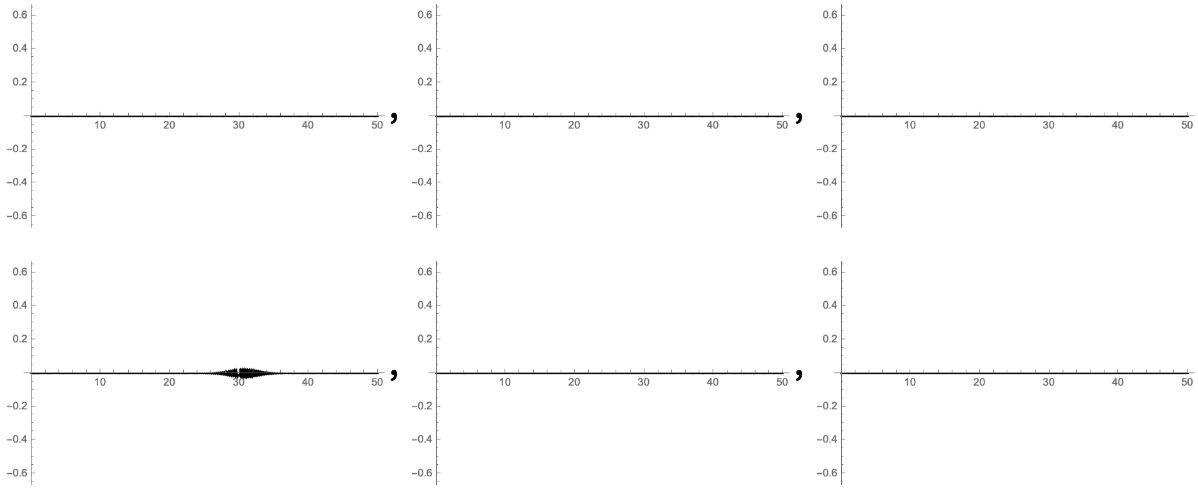


Figure 3.10: $\bar{y} = 15$, $\bar{p} = -15$.

3.3 $\bar{\mathbf{y}} = 10$

Table 3.3: Expected position of particle with $\bar{y} = 10$.

$\bar{p}$	b	$t = 1$	$t = 2$	$t = 3$
5	N/A	$q = 21$	$q = 34$	$q = 49$
0	N/A	$q = 11$	$q = 14$	$q = 19$
-5	1.12	$q = 1$	$q = 7.52$	$q = 18.02$
-10	0.51	$q = 9.47$	$q = 30.42$	$q = 53.37$
-15	0.34	$q = 19.88$	$q = 51.53$	$q = 85.18$

```
(* yb=10 pb=5 *)
```

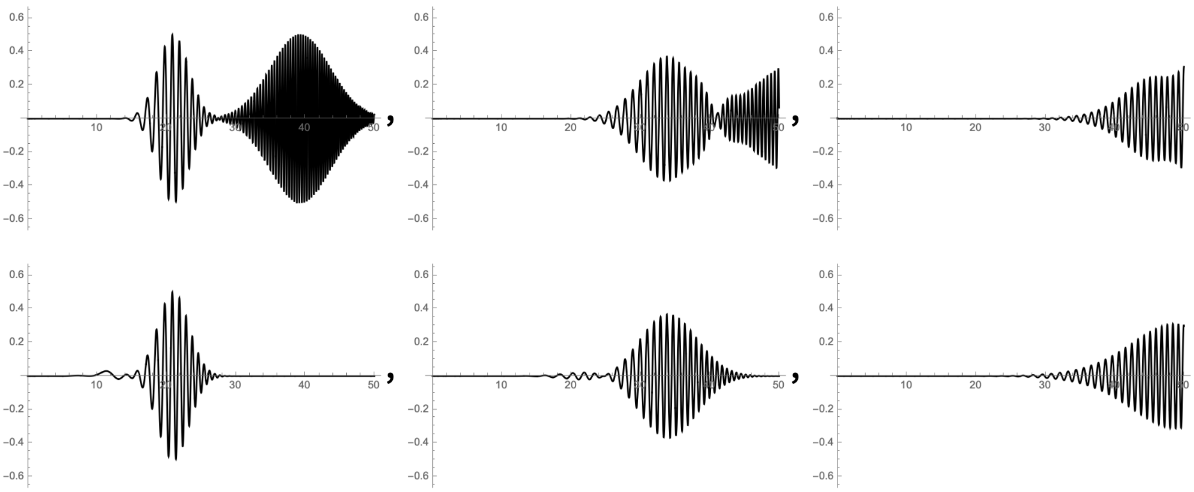


Figure 3.11: $\bar{y} = 10, \bar{p} = 5$.

```
(* yb=10 pb=0 *)
```

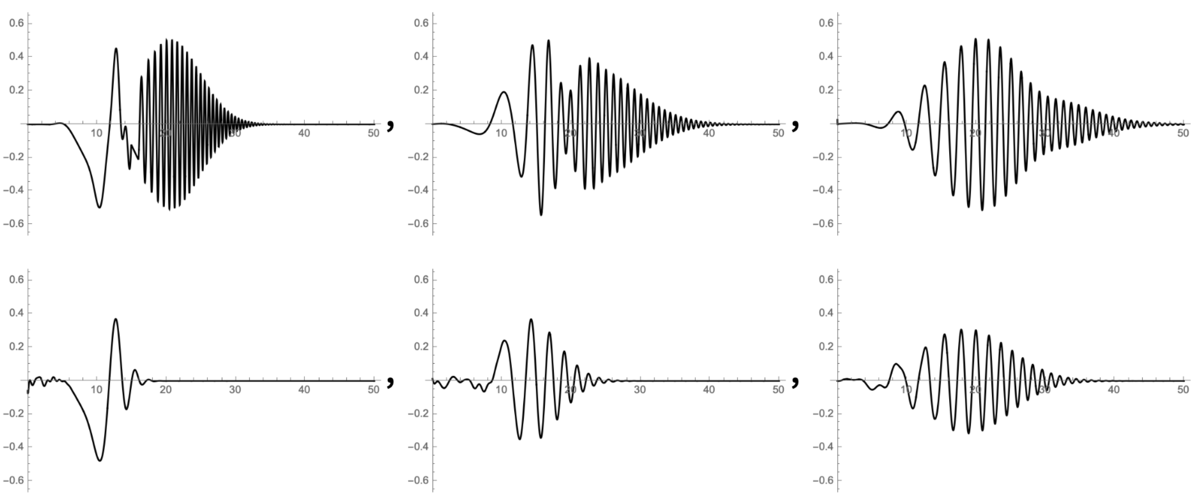


Figure 3.12: $\bar{y} = 10, \bar{p} = 0$.

```
(* yb=10 pb=-5 *)
```

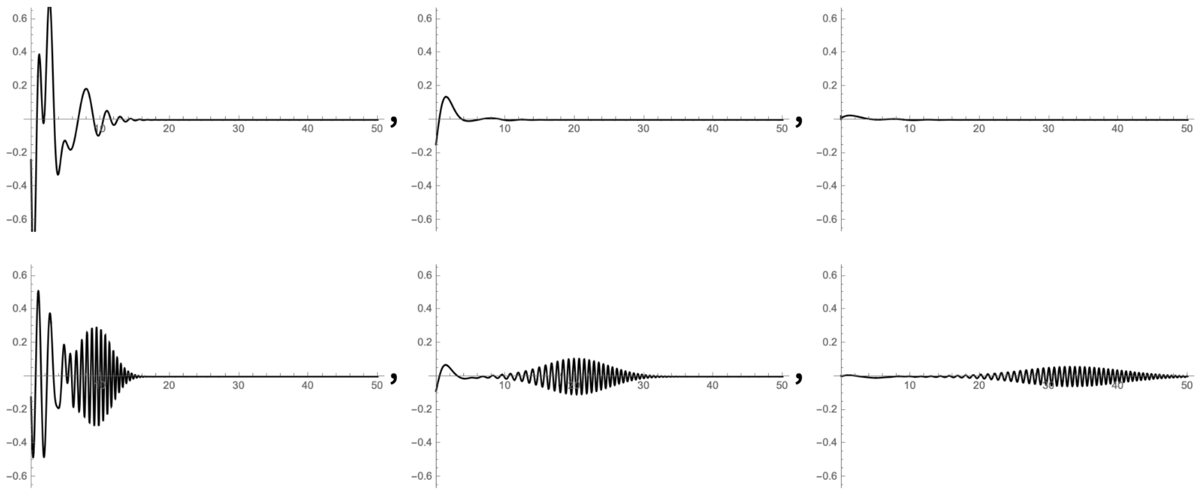


Figure 3.13: $\bar{y} = 10, \bar{p} = -5$.

```
(* yb=10 pb=-10 *)
```

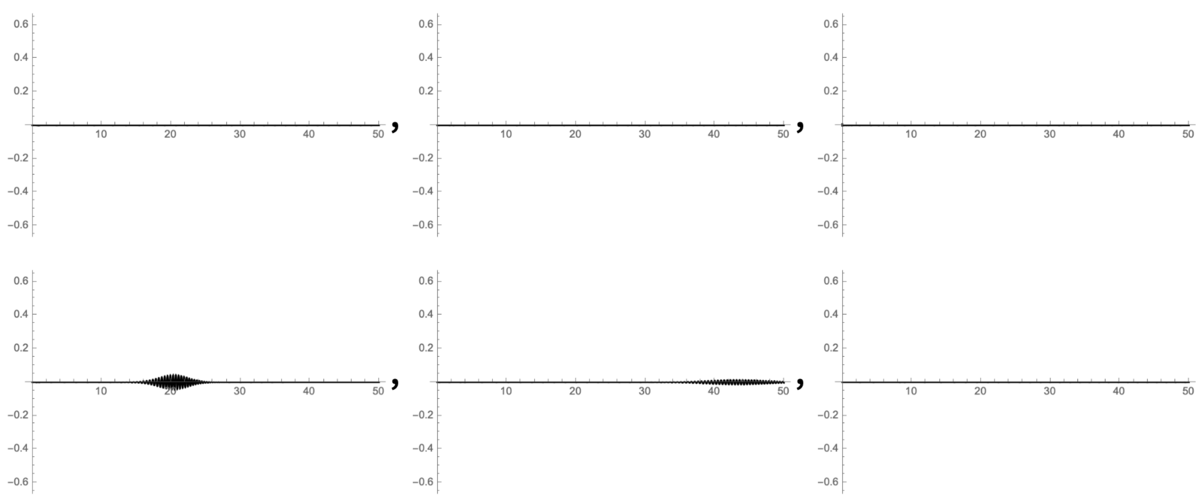


Figure 3.14: $\bar{y} = 10, \bar{p} = -10$.

```
(* yb=10 pb=-15 *)
```

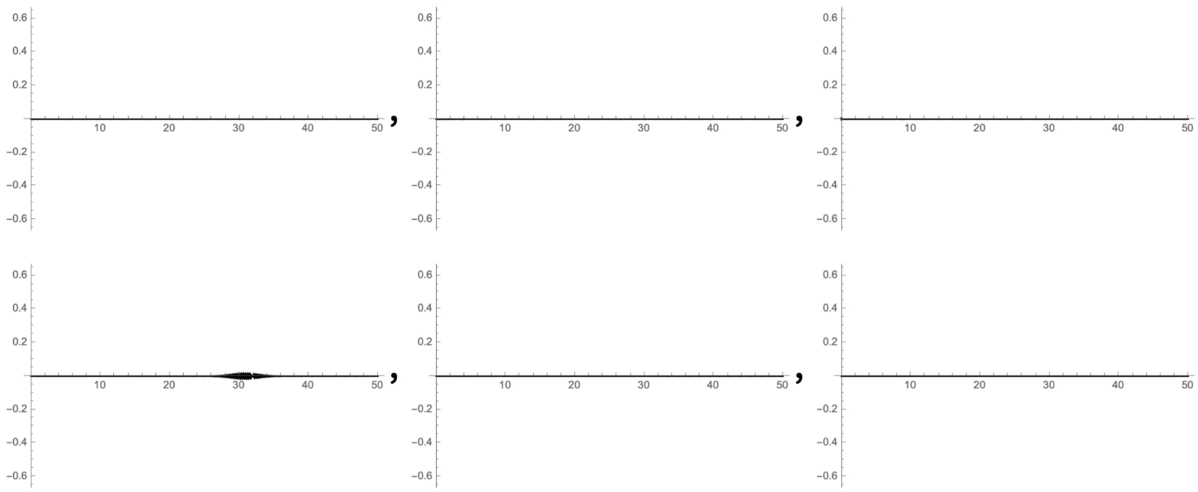


Figure 3.15: $\bar{y} = 10$, $\bar{p} = -15$.

3.4 $\bar{\mathbf{y}} = 5$

Table 3.4: Expected position of particle with $\bar{y} = 5$.

$\bar{p}$	b	$t = 1$	$t = 2$	$t = 3$
5	N/A	$q = 16$	$q = 29$	$q = 44$
0	N/A	$q = 6$	$q = 9$	$q = 14$
-5	0.53	$q = 4.45$	$q = 15.33$	$q = 28.22$
-10	0.25	$q = 15.12$	$q = 37.10$	$q = 61.09$
-15	0.17	$q = 25.39$	$q = 57.72$	$q = 92.04$

```
(* yb=5 pb=5 *)
```

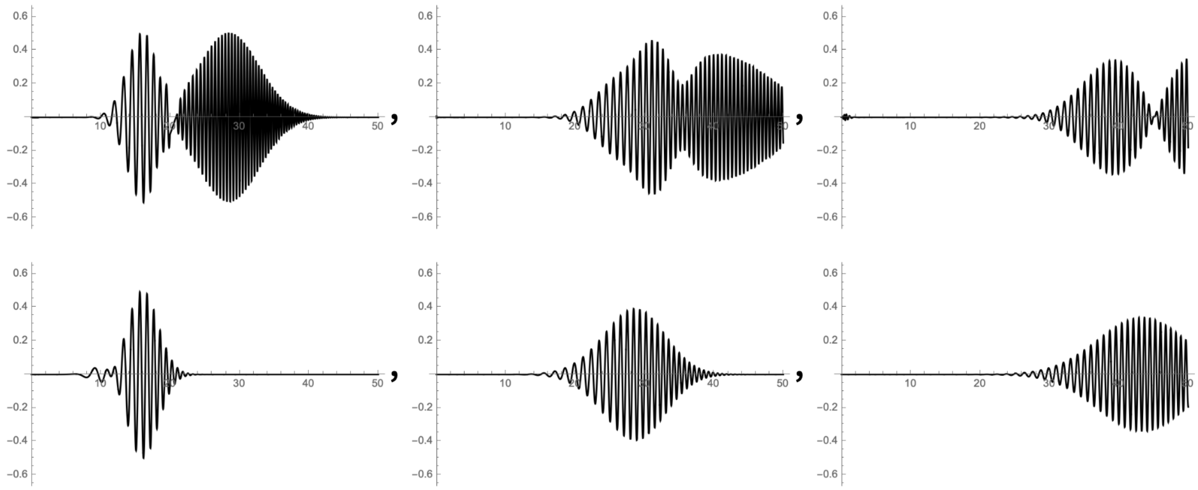


Figure 3.16: $\bar{y} = 5$, $\bar{p} = 5$.

```
(* yb=5 pb=0 *)
```

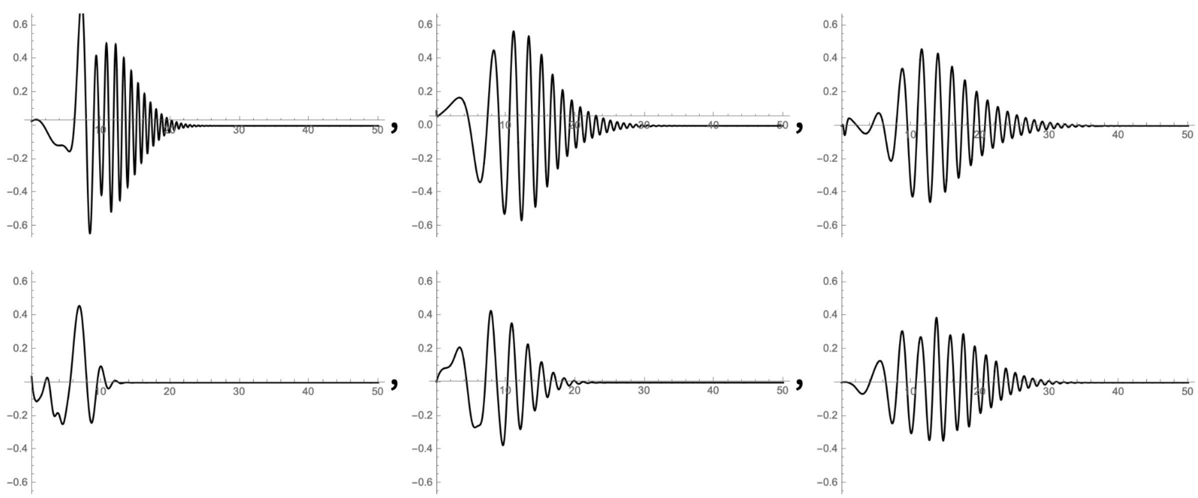


Figure 3.17: $\bar{y} = 5$, $\bar{p} = 0$.

```
(* yb=5 pb=-5 *)
```

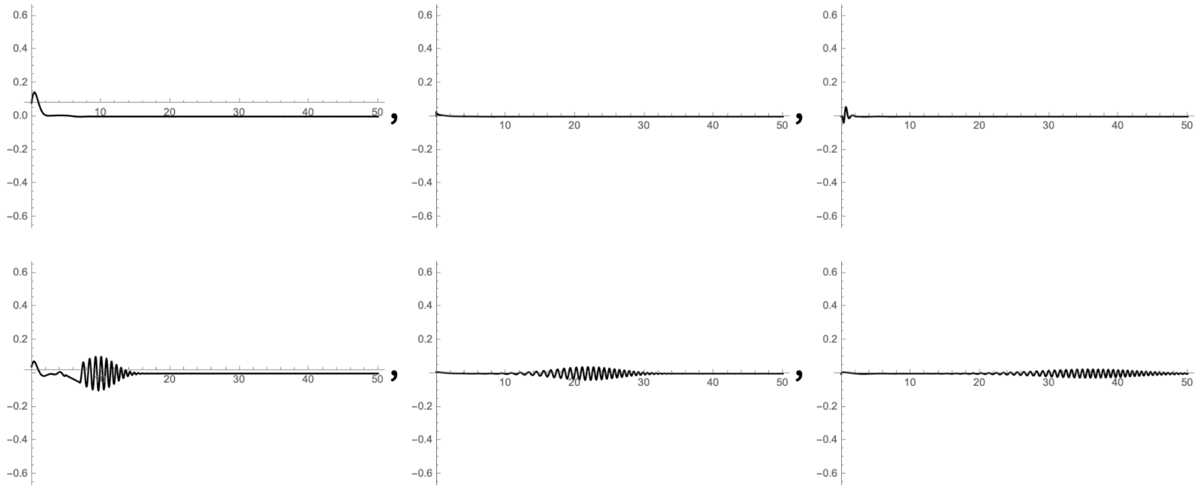


Figure 3.18: $\bar{y} = 5, \bar{p} = -5.$

```
(* yb=5 pb=-10 *)
```

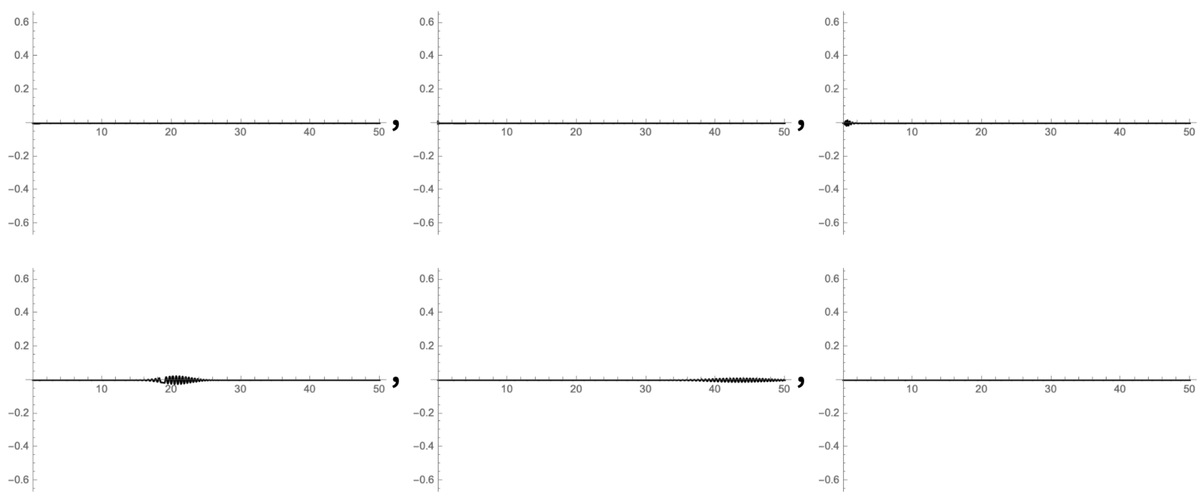


Figure 3.19: $\bar{y} = 5, \bar{p} = -10.$

```
(* yb=5 pb=-15 *)
```

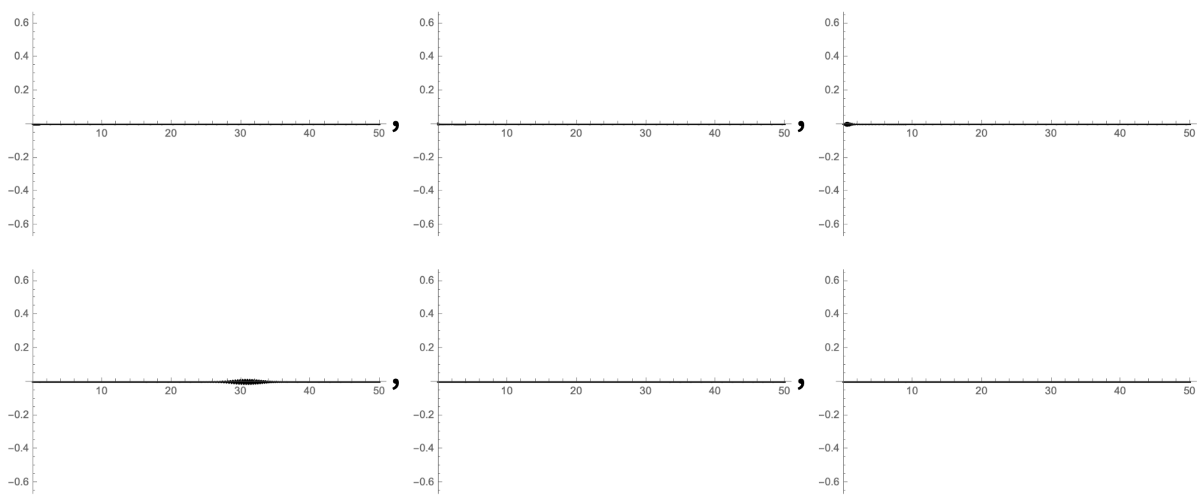


Figure 3.20: $\bar{y} = 5, \bar{p} = -15.$

4. CONCLUSION

We have successfully produced software that can be used to analyze the semiclassical picture. This software is widely applicable to other scenarios outside of the ceiling boundary case studied in this work. Moreover, we have been able to verify and correct some results of [1] including the direct path propagators (Section 1.4.2), sign convention of $\bar{p}$ in the initial Gaussian wave packets (Section 1.1.2), and have demonstrated the consistency of the addition of paths in both position and momentum space (Section 1.4.4).

4.1 Accuracy of Position Space Results

In cases in which $\bar{p} \geq 0$, the position space calculations can be seen to contain two wave packets. The leftmost wave packet is of interest and corresponds directly to the expected centroid presented in Tables 3.1, 3.2, 3.3, and 3.4. The highly oscillatory wave packet on the right is unexpected and its origin is unknown at the time of submission of this thesis. In the case of negative $\bar{p}$, we note that the both wave packets vanish (at least in the domain selected for presentation). These observations are unaffected by the value of $\bar{y}$.

4.2 Accuracy of Momentum Space Results

Momentum space calculations are favored for all values of $\bar{y}$ with $\bar{p} \geq 0$. We see from Figures 3.1, 3.2, 3.6, 3.7, 3.11, 3.12, 3.16, and 3.17 the two calculations are in agreement if the highly oscillatory wave packet to the right of the expected wave packet in the position space calculation is ignored. Because this extra wave packet is obviously an unnecessary artifact, we conclude that the momentum space calculation is favored for these values of $\bar{y}$ and $\bar{p}$. In the case of negative $\bar{p}$, we note that a highly oscillatory additional wave packet appears in the momentum space calculations. Because of the unknown origin of this artifact, the momentum space calculation should not be relied on for negative $\bar{p}$.

4.3 Constraints on Gaussian Wave Packet Data

It is believed that there is an unknown error in the bounce related wave function contributions. We see that for figures following the time of bounce, the expected wave function is absent and therefore does not correspond to the centroid calculated and presented in the related table.

We conclude that the values of $\bar{y}$ do not seem to affect any results and that the key discrepancies lie in the cases in which $\bar{p}$ is negative and a bounce has occurred. Despite the difficulties in computing the bounce related contributions, the approximation is very successful in computing cases with $\bar{p} \geq 0$. If the artifact depicted in the position space calculation is ignored, we observe that the two methods yield equivalent wave packets and correspond exactly to the expected centroid from the classical solutions. However, due to this highly oscillatory wave packet we conclude that the momentum space calculation is to be favored for all cases in which $\bar{p} \geq 0$. For negative $\bar{p}$ the position space calculation is currently favored as there are no excess wave packets, but neither case is able to reproduce the classical results for the reflected packet.

4.4 Future Goals

In future projects, we hope to determine the origin of the bounce path errors. To ensure the errors do not stem from the numerical computation, alternative software programs such as *MATLAB* or *Maple* should be used to re-derive all results presented in this paper. If results differ, than it is understood that the issue stems from the limitations of the Mathematica software. However, if results are reproduced then it is clear that the source of error must originate from an error in [1]. We believe it is the former.

REFERENCES

[1] T. A. Zapata and S. A. Fulling, "WKB propagators in position and momentum space for a linear potential with a 'ceiling' boundary," *J. Phys. A: Math. Theor.* ***50*** *105303*, 2017.

[2] A. Messiah, *Quantum Mechanics. Vol. 1.* North Holland Publishing Company, 1961.

[3] V. P. Maslov and M. V. Fedoriuk, "Semi-Classical Approximation in Quantum Mechanics," 1981.

[4] R. G. Littlejohn, "The Van Vleck formula, Maslov theory, and phase space geometry," *J. Stat. Phys.* ***68*** *7-50*, 1992.

[5] J. B. Delos, "Semiclassical calculation of quantum mechanical wave functions," *Adv. Chem. Phys.* ***65*** *161-214*, 2007.

[6] F. D. Mera, S. A. Fulling, J. D. Bouas, and K. Thapa, "WKB approximation to the power wall," *J. Phys. A: Math. Theor.* ***46*** *195302*, 2013.

APPENDIX A: TotalWaveFunction.nb


```
(* Choice of Parameters *)
YBAR := 11
PBAR := 6
TIME := 1
```

Gaussian Wavepacket

psi[y_] := $e^{i\,pb\,y-\frac{(y-yb)^2}{g}} \left(\frac{1}{g}\right)^{1/4} \left(\frac{2}{\pi}\right)^{1/4}$ (*Eq.5*)

phi[p_] := $\frac{e^{-\frac{1}{4} g\,(p-pb)^2 - i\,(p-pb)\,yb}\, g^{1/4}}{(2\,\pi)^{1/4}}$ (*Eq.6*)

Direct Propagator

Ud[y_] := $\frac{e^{i\left(\frac{2 t^3}{3}+t^2\left(-t+\frac{x-y}{t}\right)+t\left(\frac{1}{4}\left(-t+\frac{x-y}{t}\right)^2+y\right)\right)}}{2\sqrt{\pi}\,\sqrt{i\,t}}$ (*Eq.18*)

ud[p_] := $\frac{e^{-\frac{1}{3} i\,\left(3 p^2 t+t^3+3 p\,\left(t^2-x\right)-3 t\,x\right)}\,\sqrt{-\frac{i}{t}}\,\sqrt{i\,t}}{\sqrt{2\,\pi}}$ (*Eq.19*)

Bounce Propagator

```
tbounce := TIME
psifixed[y_] := psi[y] /. {t → tbounce, g → 2, yb → YBAR, pb → PBAR}
phifixed[p_] := phi[p] /. {t → tbounce, g → 2, yb → YBAR, pb → PBAR}
by := tbounce/2 + 1/Sqrt[3] * Sqrt[tbounce^2 + 2 (x + y)] *
    Sin[1/3 ArcSin[(3 * Sqrt[3] * tbounce * (y - x))/((tbounce^2 + 2 (x + y))^(3/2))]] (*Eq.23*)
bp := 1/3 (2 * tbounce - p - Sqrt[(p + tbounce)^2 + 3 x]) (*Eq.22*)
Ub[y_, x_] :=
  1/Sqrt[4 * Pi * I] * Sqrt[(y - by^2)/(-3 * tbounce * by + 2 (tbounce^2 - x - y) * by + 3 * y * tbounce)] *
   Exp[I (2/3 (by)^3 - (by)^2 (y/tbounce + by) + by (1/4 (y/tbounce + by)^2 + y))] *
   Exp[I (2/3 (tbounce - by)^3 + (tbounce - by)^2 (x/tbounce - (tbounce - by)))] *
   Exp[I ((tbounce - by)/4 (x/tbounce - (tbounce - by))^2)] (*Eq.21*)
ub[p_, x_] := -1/Sqrt[2 Pi] * Sqrt[(p + bp)/Sqrt[(p + tbounce)^2 + 3 x]] *
   Exp[I (-1/3 (bp^3 + (tbounce - bp)^3) - bp * p (3 p + 2 bp))] *
   Exp[I ((tbounce - bp) (x + (p + bp)^2))] (*Eq.20*)
```

Type I

$x \in (t^2, \infty)$

$y \in (0,\ x - t)$

$p \in \left(0,\ \frac{x - t^2}{2\,t}\right)$

```
type1y = Integrate[Ud[y] × psi[y], {y, 0, x - t^2}, Assumptions → {g > 0, t > 0}]
```

$$\frac{1}{2^{3/4}\,g^{1/4}\,\pi^{1/4}\,\sqrt{i\,t}}\,e^{\frac{t^4 - i\,g\left(3\,pb^2\,t + t^3 + 3\,pb\left(t^2 - x\right) - 3\,t\,x\right) - 3\left(x - yb\right)^2 - 12\,pb\,t\,yb - 6\,t^2\left(x + yb\right)}{3\left(g + 4\,i\,t\right)}}\; t\left(-\frac{i\,g\sqrt{-\frac{i\left(g\left(2\,pb\,t + t^2 - x\right) - 4\,i\,t\,yb\right)^2}{g\left(g + 4\,i\,t\right)t}}\;\mathrm{Erf}\!\left[\frac{1}{2}\sqrt{-\frac{i\left(g\left(2\,pb\,t + t^2 - x\right) - 4\,i\,t\,yb\right)^2}{g\left(g + 4\,i\,t\right)t}}\right]}{g\left(2\,pb\,t + t^2 - x\right) - 4\,i\,t\,yb} + \frac{\left(g\,pb - 2\,i\left(t^2 - x + yb\right)\right)\mathrm{Erf}\!\left[\sqrt{\frac{i\,t\left(i\,g\,pb + 2\left(t^2 - x + yb\right)\right)^2}{g\left(g + 4\,i\,t\right)}}\right]}{\left(g + 4\,i\,t\right)\sqrt{\frac{i\,t\left(i\,g\,pb + 2\left(t^2 - x + yb\right)\right)^2}{g\left(g + 4\,i\,t\right)}}}\right)$$

```
type1p = Integrate[ud[p] × phi[p], {p, 0, (x - t^2) / (2 t)}, Assumptions → {g > 0, t > 0}]
```

$$\frac{1}{\left(2\,\pi\right)^{3/4}}\,e^{\frac{t^4 - i\,g\left(3\,pb^2\,t + t^3 + 3\,pb\left(t^2 - x\right) - 3\,t\,x\right) - 3\left(x - yb\right)^2 - 12\,pb\,t\,yb - 6\,t^2\left(x + yb\right)}{3\left(g + 4\,i\,t\right)}}\; g^{1/4}\left(-\frac{\sqrt{\pi}\,\sqrt{\frac{\left(g\left(2\,pb\,t + t^2 - x\right) - 4\,i\,t\,yb\right)^2}{g + 4\,i\,t}}\;\mathrm{Erf}\!\left[\frac{\sqrt{\frac{\left(g\left(2\,pb\,t + t^2 - x\right) - 4\,i\,t\,yb\right)^2}{g + 4\,i\,t}}}{4\,t}\right]}{g\left(2\,pb\,t + t^2 - x\right) - 4\,i\,t\,yb} + \frac{\sqrt{\pi}\,\sqrt{\frac{\left(g\,pb - 2\,i\left(t^2 - x + yb\right)\right)^2}{g + 4\,i\,t}}\;\mathrm{Erf}\!\left[\frac{1}{2}\sqrt{\frac{\left(g\,pb - 2\,i\left(t^2 - x + yb\right)\right)^2}{g + 4\,i\,t}}\right]}{g\,pb - 2\,i\left(t^2 - x + yb\right)}\right)$$

Type II

$x \in (0, \infty)$
$y \in (x + t^2, \infty)$
$p \in (-\infty, -t)$

```
type2y = Integrate[Ud[y] × psi[y], {y, x + t^2, Infinity}, Assumptions → {g > 0, t > 0}]
```

$$\left(e^{\frac{t^4 - i g \left(3 pb^2 t + t^3 + 3 pb \left(t^2 - x\right) - 3 t x\right) - 3 \left(x - yb\right)^2 - 12 pb\, t\, yb - 6 t^2 \left(x + yb\right)}{3 \left(g + 4 i t\right)}} \left(i g \left(pb + t\right) - 2 \left(t^2 + x - yb\right) + \sqrt{-i g + 4 t} \sqrt{-\frac{i \left(g \left(pb + t\right) + 2 i \left(t^2 + x - yb\right)\right)^2}{g + 4 i t}} \operatorname{Erf}\left[\sqrt{-\frac{i t \left(g \left(pb + t\right) + 2 i \left(t^2 + x - yb\right)\right)^2}{g \left(g + 4 i t\right)}}\right]\right)\right) \Big/ \left(2^{3/4} \left(-g\right)^{1/4} \pi^{1/4} \sqrt{-i + \frac{4 t}{g}} \left(i g \left(pb + t\right) - 2 \left(t^2 + x - yb\right)\right)\right)$$

```
type2p = Integrate[ud[p] × phi[p], {p, -Infinity, -t}, Assumptions → {g > 0, t > 0}]
```

$$\left(e^{-\frac{-t^4 + i g \left(3 pb^2 t + t^3 + 3 pb \left(t^2 - x\right) - 3 t x\right) + 3 \left(x - yb\right)^2 + 12 pb\, t\, yb + 6 t^2 \left(x + yb\right)}{3 \left(g + 4 i t\right)}} g^{1/4} \left(g \left(pb + t\right) + 2 i \left(t^2 + x - yb\right) - \sqrt{g + 4 i t} \sqrt{\frac{\left(g \left(pb + t\right) + 2 i \left(t^2 + x - yb\right)\right)^2}{g + 4 i t}} \operatorname{Erf}\left[\frac{1}{2} \sqrt{\frac{\left(g \left(pb + t\right) + 2 i \left(t^2 + x - yb\right)\right)^2}{g + 4 i t}}\right]\right)\right) \Big/ \left(2^{3/4} \pi^{1/4} \sqrt{g + 4 i t} \left(g \left(pb + t\right) + 2 i \left(t^2 + x - yb\right)\right)\right)$$

Type III (a)

$x \in (0, t^2)$

$y \in ((\sqrt{x} - t)^2, x + t^2)$

$p \in (-t, -\sqrt{x} - t)$

```
type3ay =
 Integrate[Ud[y] × psi[y], {y, (Sqrt[x] - t)^2, x + t^2}, Assumptions → {g > 0, t > 0}]
```

$$\frac{1}{2^{3/4} g^{1/4} \pi^{1/4} \sqrt{i t}} e^{\frac{t^4 - i g \left(3 pb^2 t + t^3 + 3 pb (t^2 - x) - 3 t x\right) - 3 (x - yb)^2 - 12 pb\, t\, yb - 6 t^2 (x + yb)}{3 (g + 4 i t)}} \left(\frac{i g \sqrt{-\frac{i t \left(g (pb + t) + 2 i (t^2 + x - yb)\right)^2}{g (g + 4 i t)}}\ \mathrm{Erf}\left[\sqrt{-\frac{i t \left(g (pb + t) + 2 i (t^2 + x - yb)\right)^2}{g (g + 4 i t)}}\right]}{g (pb + t) + 2 i (t^2 + x - yb)} - \frac{i \sqrt{-\frac{i g t \left(g (pb + t - \sqrt{x}) + 2 i (t^2 - 2 t \sqrt{x} + x - yb)\right)^2}{g + 4 i t}}\ \mathrm{Erf}\left[\sqrt{\frac{i t \left(i g (pb + t - \sqrt{x}) - 2 (t^2 - 2 t \sqrt{x} + x - yb)\right)^2}{g (g + 4 i t)}}\right]}{g (pb + t - \sqrt{x}) + 2 i (t^2 - 2 t \sqrt{x} + x - yb)} \right)$$

```
type3ap = Integrate[ud[p] × phi[p], {p, -t, Sqrt[x] - t}, Assumptions → {g > 0, t > 0}]
```

$$\frac{1}{2^{3/4} \pi^{1/4}} e^{\frac{t^4 - i g \left(3 pb^2 t + t^3 + 3 pb (t^2 - x) - 3 t x\right) - 3 (x - yb)^2 - 12 pb\, t\, yb - 6 t^2 (x + yb)}{3 (g + 4 i t)}} g^{1/4} \left(\frac{\sqrt{\frac{\left(g (pb + t) + 2 i (t^2 + x - yb)\right)^2}{g + 4 i t}}\ \mathrm{Erf}\left[\frac{1}{2} \sqrt{\frac{\left(g (pb + t) + 2 i (t^2 + x - yb)\right)^2}{g + 4 i t}}\right]}{g (pb + t) + 2 i (t^2 + x - yb)} - \frac{\sqrt{\frac{\left(g (pb + t - \sqrt{x}) + 2 i (t^2 - 2 t \sqrt{x} + x - yb)\right)^2}{g + 4 i t}}\ \mathrm{Erf}\left[\frac{1}{2} \sqrt{\frac{\left(g (pb + t - \sqrt{x}) + 2 i (t^2 - 2 t \sqrt{x} + x - yb)\right)^2}{g + 4 i t}}\right]}{g (pb + t - \sqrt{x}) + 2 i (t^2 - 2 t \sqrt{x} + x - yb)} \right)$$

Type III (b)

$x \in (t^2, \infty)$

$y \in (x - t^2, x + t^2)$

p: $(-t, 0)$

```
type3by = Integrate[Ud[y] × psi[y], {y, x - t^2, x + t^2}, Assumptions → {g > 0, t > 0}]
```

$$-\Bigg(\Bigg((-1)^{3/4}\, e^{-\frac{-t^4+i g \left(3 pb^2 t+t^3+3 pb \left(t^2-x\right)-3 t x\right)+3 (x-yb)^2+12 pb\, t\, yb+6 t^2 (x+yb)}{3 (g+4 i t)}}\, g^{1/4} \Bigg(i (g+4 i t)\, t \sqrt{-\frac{i \left(g (pb+t)+2 i \left(t^2+x-yb\right)\right)^2}{g+4 i t}} \sqrt{\frac{i \left(i g\, pb+2 \left(t^2-x+yb\right)\right)^2}{g+4 i t}}\, \mathrm{Erf}\left[\sqrt{-\frac{i t \left(g (pb+t)+2 i \left(t^2+x-yb\right)\right)^2}{g (g+4 i t)}}\right] - t \left(g^2 pb (pb+t)+4 \left(t^4-(x-yb)^2\right)-2 i g \left(t^3+2 pb (-x+yb)+t (-x+yb)\right)\right) \mathrm{Erf}\left[\sqrt{\frac{i t \left(i g\, pb+2 \left(t^2-x+yb\right)\right)^2}{g (g+4 i t)}}\right]\Bigg)\Bigg) \Big/ \left(2^{3/4} \pi^{1/4} (g+4 i t)\, t \left(g (pb+t)+2 i \left(t^2+x-yb\right)\right) \sqrt{\frac{i \left(i g\, pb+2 \left(t^2-x+yb\right)\right)^2}{g+4 i t}}\right)\Bigg)$$

```
type3bp = Integrate[ud[p] × phi[p], {p, -t, 0}, Assumptions → {g > 0, t > 0}]
```

$$\frac{1}{(2\pi)^{3/4}}\, e^{\frac{t^4-i g \left(3 pb^2 t+t^3+3 pb \left(t^2-x\right)-3 t x\right)-3 (x-yb)^2-12 pb\, t\, yb-6 t^2 (x+yb)}{3 (g+4 i t)}}\, g^{1/4} \left(\frac{\sqrt{\pi} \sqrt{\frac{\left(g (pb+t)+2 i \left(t^2+x-yb\right)\right)^2}{g+4 i t}}\, \mathrm{Erf}\left[\frac{1}{2} \sqrt{\frac{\left(g (pb+t)+2 i \left(t^2+x-yb\right)\right)^2}{g+4 i t}}\right]}{g (pb+t)+2 i \left(t^2+x-yb\right)} - \frac{\sqrt{\pi} \sqrt{\frac{\left(g\, pb-2 i \left(t^2-x+yb\right)\right)^2}{g+4 i t}}\, \mathrm{Erf}\left[\frac{1}{2} \sqrt{\frac{\left(g\, pb-2 i \left(t^2-x+yb\right)\right)^2}{g+4 i t}}\right]}{g\, pb-2 i \left(t^2-x+yb\right)}\right)$$

Direct I

```
direct1y := (type2y + type3ay) /. {t → TIME, g → 2, yb → YBAR, pb → PBAR}
direct1p := (type2p + type3ap) /. {t → TIME, g → 2, yb → YBAR, pb → PBAR}
```

Direct II

```
direct2y := (type1y + type2y + type3by) /. {t → TIME, g → 2, yb → YBAR, pb → PBAR}
direct2p := (type1p + type2p + type3bp) /. {t → TIME, g → 2, yb → YBAR, pb → PBAR}
```

Bounce a

$x \in (0, t^2)$

$y \in ((t - \sqrt{x})^2, \infty)$

$p \in (-\infty, \sqrt{x} - t)$

```
bounceay := NIntegrate[Ub[y, x] × psifixed[y], {y, (tbounce - Sqrt[x]) ^2, Infinity}]
bounceap := NIntegrate[ub[p, x] × phifixed[p], {p, -Infinity, Sqrt[x] - tbounce}]
```

Bounce b

$x \in (t^2, \infty)$

$y \in (0, \infty)$

$p \in (-\infty, \frac{t^2 - x}{2t})$

```
bounceby := NIntegrate[Ub[y, x] × psifixed[y], {y, 0, Infinity}]
bouncebp := NIntegrate[ub[p, x] * phifixed[p], {p, -Infinity, (tbounce^2 - x)/(2 * tbounce)}]
```

[x < t^2]

```
final1y =
 Plot[Re[direct1y + bounceay], {x, 0, TIME^2}, PlotRange → Full, PlotStyle → Black]
```

```
final1p =
 Plot[Re[direct1p + bounceap], {x, 0, TIME^2}, PlotRange → Full, PlotStyle → Black]
```

[x > t^2]

```
final2y =
 Plot[Re[direct2y + bounceby], {x, TIME^2, 40}, PlotRange → Full, PlotStyle → Black]
```

```
final2p =
 Plot[Re[direct2p + bouncebp], {x, TIME^2, 40}, PlotRange → Full, PlotStyle → Black]
```

Complete Wave Packet

```
PSIY = Show[final1y, final2y, PlotRange → {-0.6, 0.6}](*Eq.3*)
```

```
PSIP = Show[final1p, final2p, PlotRange → {-0.6, 0.6}](*Eq.4*)
```

APPENDIX B: Free.nb

Gaussian Wavepacket

$$\text{psi[y\_] := } e^{i\,pb\,y - \frac{(y-yb)^2}{g}} \left(\frac{1}{g}\right)^{1/4} \left(\frac{2}{\pi}\right)^{1/4} \text{(*Eq.5*)}$$

$$\text{phi[p\_] := } \frac{e^{-\frac{1}{4} g\,(p-pb)^2 - i\,(p-pb)\,yb}\, g^{1/4}}{(2\,\pi)^{1/4}} \text{(*Eq.6*)}$$

Free Propagator

$$\text{uf[p\_] := } \frac{e^{-i\,p^2\,t + i\,p\,x}}{\sqrt{2\,\pi}} \text{(*Eq.16*)}$$

$$\text{Uf[y\_] := } \frac{e^{\frac{i\,(x-y)^2}{4\,t}}}{2\,\sqrt{\pi}\,\sqrt{i\,t}} \text{(*Eq.17*)}$$

Free Particle

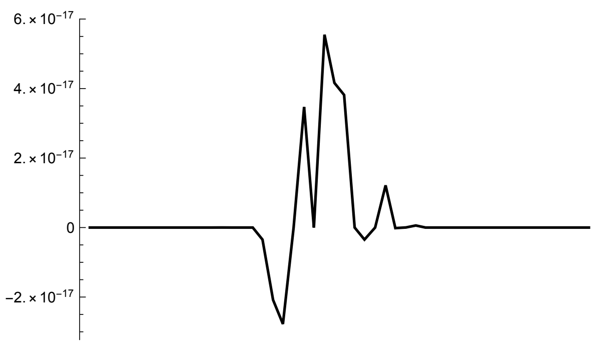
```
freey = Integrate[Uf[y] × psi[y], {y, -Infinity, Infinity}, Assumptions → {g > 0, t > 0}]
```

$$\frac{e^{-\frac{i\, g\, pb\, (pb\, t - x) + x^2 - 2\, x\, yb + yb\, (4\, pb\, t + yb)}{g + 4\, i\, t}} \left(\frac{2}{\pi}\right)^{1/4}}{g^{1/4} \sqrt{\frac{4}{g} - \frac{i}{t}}\ \sqrt{i\, t}}$$

```
freep = Integrate[uf[p] × phi[p], {p, -Infinity, Infinity}, Assumptions → {g > 0, t > 0}]
```

$$\frac{e^{-\frac{i\, g\, pb\, (pb\, t - x) + (x - yb)^2 + 4\, pb\, t\, yb}{g + 4\, i\, t}}\, g^{1/4} \left(\frac{2}{\pi}\right)^{1/4}}{\sqrt{g + 4\, i\, t}}$$

```
test = Plot[Re[freey - freep] /. {t → 1, g → 2, yb → 11, pb → 6},
  {x, 1, 50}, PlotRange → Full, PlotStyle → Black]
```

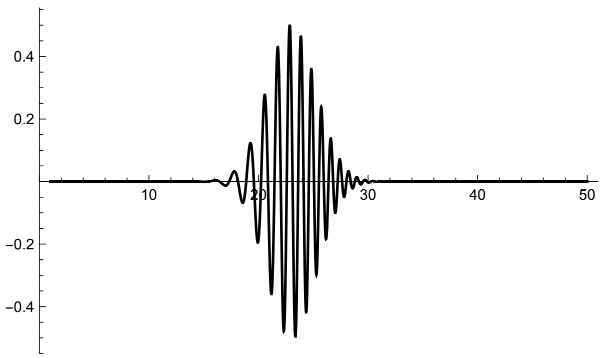



```
(*Both are equivalent so we rename it as free*)
```

$$\text{free}[x\_, t\_, g\_, yb\_, pb\_] := \frac{(1 - i)\, e^{-\frac{i\, g\, pb\, (pb\, t - x) + (x - yb)^2 + 4\, pb\, t\, yb}{g + 4\, i\, t}}\, g^{1/4}}{(2\, \pi)^{1/4} \sqrt{-i\, g + 4\, t}}$$

Dynamics of Free Particle

```
PSI = Plot[Re[free[x, t, g, yb, pb]] /. {t → 1, g → 2, yb → 11, pb → 6},
  {x, 1, 50}, PlotRange → Full, PlotStyle → Black]
```




```
PSIDynamic = Manipulate[
  Plot[Re[free[x, t, g, yb, pb] /. {g → 2}], {x, 1, 50}, PlotRange → {-0.6, 0.6},
   PlotStyle → Black], {t, 1, 3, 1}, {yb, 0, 20, 1}, {pb, -15, 5, 1}]
```