THE WKB APPROXIMATION FOR A

LINEAR POTENTIAL AND CEILING

A Thesis

by

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ABSTRACT

The WKB Approximation for a

Linear Potential and Ceiling. (December 2007)

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The physical problem this thesis deals with is a quantum system with linear potential driving a particle away from a ceiling (impenetrable barrier). This thesis will construct the WKB approximation of the quantum mechanical propagator. The application of the approximation will be for propagators corresponding to both initial momentum data and initial position data.

Although the analytic solution for the propagator exists, it is an indefinite integral of Airy functions and difficult to use in obtaining probability densities by numerical integration or other schemes considered by the author. The WKB construction is less problematic because it is representable in exact form, and integration schemes (both numerical and analytic) to obtain probability densities are straightforward to implement. Another purpose of this thesis is to be a starting point for the construction of WKB propagators with general potentials but the same type of boundary, impenetrable barrier.

Research pertaining to this thesis includes determining all classical paths and constraints for the one-dimensional linear potential with ceiling, and using these equations to construct the classical action, and hence the WKB approximation. Also, evaluation of final quantum wave functions using numerical integration to check and better understand the approximation is part of the research.

The results indicate that the validity of the WKB approximation depends on the type of classical paths (i.e. the initial data of the path) used in the construction.

Specifically, the presence of the ceiling may cause the semi-classical wave packets to become vanishingly small in one representation of initial classical data, while not effecting the packets in another. The conclusion of this phenomenon is that the representation where the packets are not annihilated is the correct representation.

To Mom and Dad, I love you very much.

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I give all thanks and praise to Jesus Christ for the knowledge I have been blessed with, and the men and women whom have guided me throughout this life.

Special thanks go to Dr. Stephen A. Fulling for taking me in as a beginner, and never giving up on me, for listening to my crazy ideas with respect and having confidence in my abilities, and for sharing his ingenious views of nature with me.

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INTRODUCTION

Use of the ansatz

$$\psi(x,\lambda) = e^{\frac{i}{\lambda}S(x)}\sum_{j=0}^{\infty}(\frac{i}{\lambda})^{-j}A_j(x) \tag{1.1}$$
$$\lambda \rightarrow \infty$$

to solve differential equations has been in circulation since the mid-nineteenth century [1]. In 1911 P. Debye used (1.1) for the solution of partial differential equations. Soon after Debye's work the physicists Wentzel, Kramers, Brillouin, and the English mathematician Jeffreys used this technique to solve the Schrödinger equation

$$\frac{-\hbar^2}{2m}\nabla^2\psi + V(\vec{x})\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{1.2}$$

For this situation the parameter λ in (1.1) becomes Planc's constant, $\hbar$. The solutions of the Schrödinger equation using the ansatz (1.1) are equivalent to the solutions of the Feynman Kernel

$$K(x,t) = \int D[x(t)]\, e^{\frac{i}{\hbar}S[x(t)]} \tag{1.3}$$

using the method of stationary phase [2]. For the propagator the WKB analysis is in exact agreement with the analytic solutions corresponding to the free-particle, linear potential and the quadratic potential [3]. However, the approximation is not exact for the solution of the individual wave functions of (1.2) [4].

Application of (1.1) to the Schrödinger equation yields the Hamilton-Jacobi equation of classical mechanics in association with the lowest order of $\hbar$. The corresponding

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solution is the action, $S[q(t)]$. This solution depends on the trajectories, $q(t)$, associated with the classical situation requiring both initial and final data, not the usual initial-value problem we encounter in undergraduate mechanics. However, in classical mechanics not all final data is accessible for trajectories with given initial data, and the propagator associated with such "forbidden" regions will give no information about the final probability. However, these regions may be accessible for given initial momentum data. This type of behavior, where one representation is phase space produces different results than another, is generally due to caustics ([5], [1]), or where a caustic is the limiting case of the classical trajectories. Also, the solution to the second lowest order equation in $\hbar$ (the "Amplitude") generally develops singularities by diverging as the classical trajectories pass a caustic[5]. Therefore, simply because the WKB analysis with respect to certain initial data yields a null result does not necessarily mean the propagator is also negligible. The WKB approximation corresponding to initial momentum and position data is therefore a logical analysis to partake in, which is the main motivation of this thesis.

The remainder of the Introduction will discuss aspects of the classical system, including the general constraints on a particle's initial data given final position and time. Explicit application of the WKB ansatz will follow, giving the equations governing the approximation to $\mathcal{O}(\hbar)$, and a brief overview of Hamilton-Jacobi theory. It also displays the analytic solution without derivation, and discusses the Fourier transform relationship between the momentum and position space propagators.

The second and third chapters explicitly construct the approximations corresponding to systems given initial position and momentum data, respectively. The chapters also derive the classical equations of motion and the constraints on the classical paths.

The final chapter will compare the WKB propagators in the aforementioned

Linear Potential with Barrier

∞

Ceiling

q
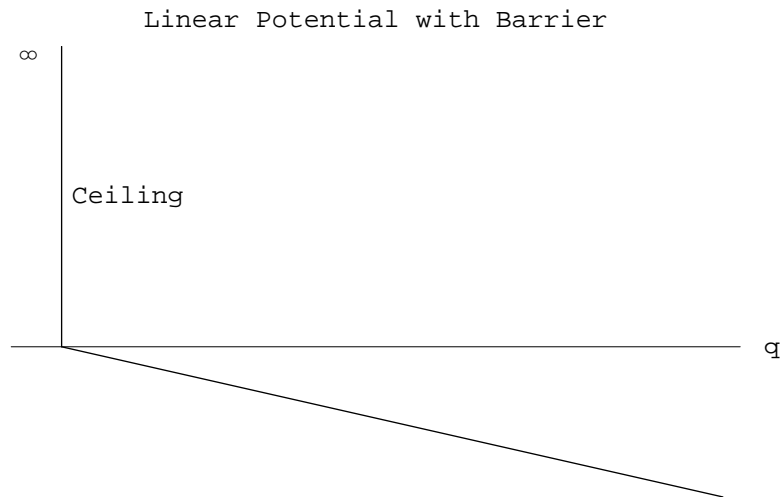
Fig. 1. The potential energy as a function of position. The ceiling is located at the origin, the ∞ highlights the fact that the origin is impenetrable to the particle (both classical and quantum).

"forbidden" region, and other cases of final data.

A. The Quantum and Classical System

The system considered in this paper is a particle confined to the positive region of a one-dimensional coordinate system by means of an impenetrable barrier at the origin, in the presence of a linear potential (cf. figure 1),

$$V(q) = -\alpha q. \tag{1.4}$$

Here q represents the position of the particle, and α characterizes the strength and direction of the potential. For α greater than zero the barrier is a "ceiling" and the particle may bounce off at most once. If α is less than zero then the barrier will act as a floor, and will have, in principle, an infinite number of bounces. This paper will consider only the ceiling case.

The Quantum theory of the system under consideration has the exact solution

in terms of the energy eigenfunctions $u(x, E)$:

$$U(x, y, t) = \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}Et} u(x, E) u(y, E) \rho(E) dE, \tag{1.5}$$

here $u(x, E)$ and $\rho(E)$ are:

$$
\begin{aligned}
u(x, E) &= \pi \left[\mathrm{Ai} \left[\lambda \left(-x - \frac{E}{\alpha} \right) \right] \mathrm{Bi} \left(-\lambda \frac{E}{\alpha} \right) \right] \\
&\quad - \pi \left[\mathrm{Bi} \left[\lambda \left(-x - \frac{E}{\alpha} \right) \right] \mathrm{Ai} \left(-\lambda \frac{E}{\alpha} \right) \right] \tag{1.6}
\end{aligned}
$$

$$\rho(E) = \frac{\pi^{-2}}{\mathrm{Ai}^2 \left(-\lambda \frac{E}{\alpha} \right) + \mathrm{Bi}^2 \left(-\lambda \frac{E}{\alpha} \right)} \tag{1.7}$$

$$\lambda \equiv \left(\frac{2m\alpha}{\hbar^2} \right)^{\frac{1}{3}}. \tag{1.8}$$

E is the energy eigenvalue of the system, t is the time of propagation, x and y are the final and initial positions, respectively. This solution is a special case of the methods considered in Dean and Fulling [6]. The evolution of an initial wave packet, $\psi(y)$, is:

$$\Psi(x, t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}Et} \psi(y) u(x, E) u(y, E) \rho(E) dE dy. \tag{1.9}$$

The analytic solution for the propagator is difficult to use in obtaining probability densities by numerical integration or other schemes. However, the WKB construction is less problematic because it is representable in exact form, and integration schemes (both numerical and analytic) to obtain probability densities are straight forward to implement.

There are two types of classical trajectories to consider: those which will bounce off the ceiling (bounce paths) and those which will not (direct paths). The latter trajectories may either initially move toward the ceiling or initially move away, corresponding to the initial momentum being less than or greater than zero, respectively. This paper will consider the trajectories corresponding to two different types of initial

data:

- Initial momentum, p, and final position, x;

- Initial position, y, and final position, x.

The equation governing the dynamics of the classical system is:

$$
\begin{aligned}
\frac{d^2 q}{d\tau^2} &= \frac{\alpha}{m} \Rightarrow \\
q(\tau) &= \frac{\alpha}{2m}\tau^2 + A\tau + B.
\end{aligned}
\tag{1.10}
$$

The constants of integration, A and B, are determined from the chosen initial conditions. For bounce trajectories two solutions are required, $q_1(\tau)$ and $q_2(\tau)$, corresponding to the dynamics before and after the collision, respectively. A third condition must be placed on the bounce trajectories such that the momenta of the paths at the ceiling is equal in magnitude and opposite in direction. Letting b denote the time at which the particle will ricochet, this condition is written as:

$$
p_1(b) = -p_2(b).
\tag{1.11}
$$

Since the classical direct paths will never interact with the ceiling, the corresponding WKB solutions for both types of data will be in agreement with the quantum system corresponding to the Hamiltonian with a linear potential without the boundary condition at the origin:

$$
\begin{aligned}
K_-(x, y, t) &= \sqrt{\frac{m}{2\pi i t \hbar}} e^{\frac{-i\alpha^2 t^3}{24 m \hbar}} e^{\frac{i\alpha t(x+y)}{2\hbar}} e^{\frac{im(x-y)^2}{2t\hbar}}
\tag{1.12} \\
\hat{K}_-(x, p, t) &= \frac{1}{\sqrt{2\pi\hbar}} e^{-i\frac{\alpha^2 t^3}{6m\hbar}} e^{\frac{i}{\hbar}(p+\alpha t)(x - \frac{pt}{2m})},
\tag{1.13}
\end{aligned}
$$

(see [2] for equation 1.12). The only discrepancy is the WKB solutions carry constraints on the initial data to ensure the particle will not interact with the ceiling. However, the WKB propagators corresponding to bounce trajectories will not yield

results identical to the analytic propagator. This is in contrast to the consensus that the WKB approximation is exact for all potentials with at most quadratic form.

The remainder of the paper will use the following units:

$$\hbar \equiv 1$$
$$m \equiv \frac{1}{2}$$
$$\alpha \equiv 1.$$

Note that in consequence of the above units, position will have the same dimensionality as time squared, and momentum will have the same dimensionality as time:

$$[x] = [t]^2$$
$$[p] = [t].$$

B. The Classical Solutions

The preliminary quest is to determine all possible trajectories, $q(\tau)$, which obey Hamilton's equations connecting the initial data $(p/y, t_0)$ with the final data (x, t). For notational simplicity the general data corresponding to the initial position and initial momentum trajectories will be:

$$\mathbf{x}_y \equiv (y, t_0), (x, t)$$
$$\mathbf{x}_p \equiv (p, t_0), (x, t).$$

There are three types of non-bounce trajectories to consider:

1. Trajectories which initially and finally move away from the ceiling: $p_0 \in (0, \infty)$, and $p_f \in (0, \infty)$

2. Trajectories which initially and finally move toward the ceiling: $p_0 \in (-\infty, 0)$,
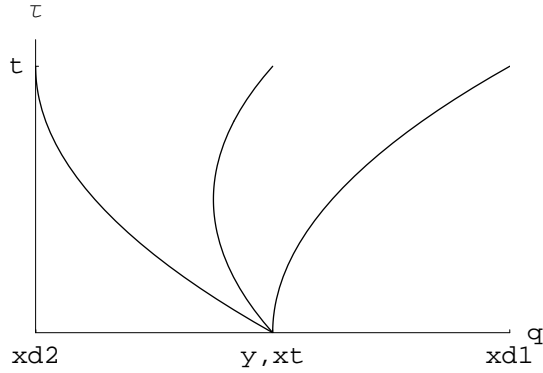
Fig. 2. Three types of non-bounce trajectories with equal initial data, y, and final time, t. The only variable is the final position, x. $xd1$ represents the final position of a type (1) trajectory. $xd2$ is the final position for type (2). And xt is for a turning trajectory, type (3).

and $p_f \in (-\infty, 0)$

3. Trajectories which initially move toward the ceiling, and end moving away from the ceiling: $p_0 \in (-\infty, 0)$, and $p_f \in (0, \infty)$

A plot of the three types of non-bounce trajectories is in figure (2). The time at which the particle's momentum is zero, n, governs the transition between motion toward the ceiling and away from the ceiling for type (3) trajectories.

There are certain fundamental or "critical" trajectories which are helpful in analyzing the more general situations. The critical trajectories of type (1) and (2) have relationships with the case where the initial momentum of the particle is zero. For given final data, (x, t), such a trajectory has initial position $\tilde{y} \equiv x - t^2$, and the trajectory is:

$$q(\tau) = \tau^2 + x - t^2. \tag{1.14}$$

Therefore, an initial relationship for this trivial case is that if $x > t^2$ the initial position will be on the physical side of the ceiling. Conversely, for $x < t^2$ the initial

position will not be physical. Keeping the same final data implies that if an initial positive momentum is given to this trajectory, the initial position must move towards the ceiling. Conversely, for an initial negative momentum the initial position must move away from the ceiling. Therefore, a general statement for the system (1.14) corresponding to trajectories of type (1) and (2) is that as the particle is given initial positive momentum the initial position must move away from the critical position, $\tilde{y}$, and towards the ceiling. Whereas for the particle to have initial negative momentum the initial position must move away from the critical position and away from the ceiling,

$$\text{Type}(1) \quad : \quad y < \tilde{y} \tag{1.15}$$

$$\text{Type}(2) \quad : \quad y > \tilde{y}. \tag{1.16}$$

The linear potential implies that the momentum gained by the particle is equal to the time of flight, τ, and the total momentum of the trajectory at any time is given by:

$$\tau + p_0,$$

where p_0 is the initial momentum of the trajectory. Therefore, the time at which the particle will turn around is:

$$n = -p_0. \tag{1.17}$$

The "boundary" between cases (2) and (3) is analyzable in terms of the distance traveled, Δ. For a trajectory where $t = n$:

$$\begin{aligned} \Delta &= -\int_0^n v(\tau)d\tau = -2\int_0^{-p_0} (p_0 + \tau)\, d\tau \Rightarrow \\ \Delta &= p_0^2 = t^2. \end{aligned} \tag{1.18}$$
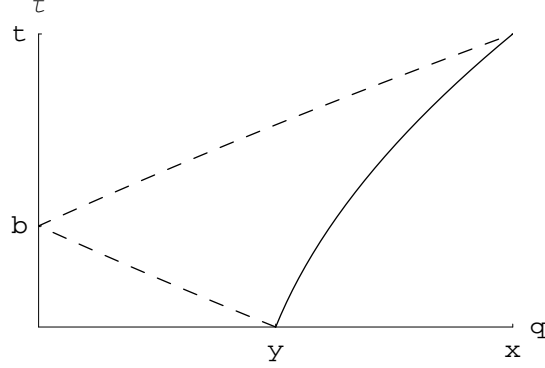
Fig. 3. General direct (solid line) and bounce (dotted line) trajectory connecting initial data, y, to the final data, x, in the same time, t.

The negative sign is placed in front of the integral because the velocity is inherently negative. In accordance with $\tilde{y}$ being the critical position for trajectories of type (1) and (2), Δ is the critical displacement for trajectories of type (3).

Some initial and final data characterize a non-bounce trajectory and a more "energetic" bounce trajectory, cf. figure (3). The critical trajectory for the bounce paths are the type (3) trajectories with zero momentum at the ceiling, corresponding to zero energy, cf. figure (4). All subsequent trajectories for the bounce case will have energy greater than zero (the proof follows in the subsequent chapters). A way to view the construction of bounce trajectories is by joining two trajectories at the ceiling which there obey equation (1.11). The trajectory prior to the bounce satisfies the initial data, and the ricochet trajectory will satisfy the final data. The critical trajectory for the bounce case is when these two trajectories are the same. A particle in a linear potential beginning at the ceiling with zero energy (and therefore zero initial momentum) will end at location x with momentum $\sqrt{x}$. Conversely, if the particle begins at y with zero energy then the momentum at the the ceiling will be $\sqrt{y}$. Therefore, the total momentum the particle will gain for the critical bounce
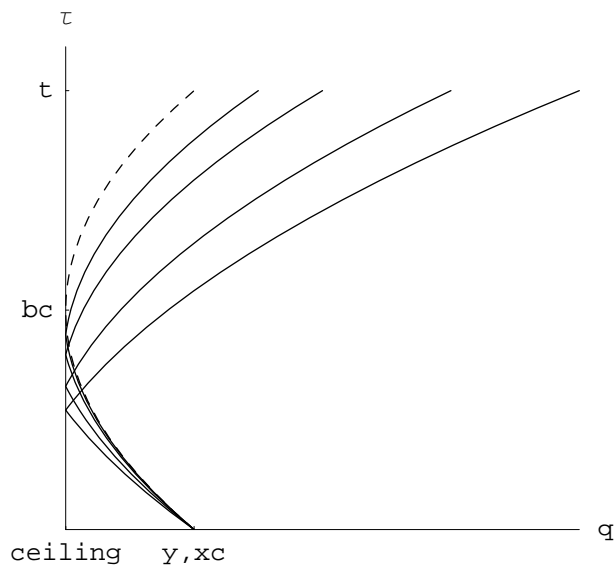
Fig. 4. Generic family of bounce trajectories with the same initial position and final time. The final position, x, is varying. The critical trajectory is dashed, and bc denotes the time of bounce for this trajectory, xc denotes the final position.

trajectory is:

$$\sqrt{x} + \sqrt{y} = t, \tag{1.19}$$

where the equality to the total time is due to the fact that the particle will gain momentum linearly with time.

C. The WKB Ansatz

The equations in this section will use $\hbar$ and m for notational clarity. The quantum mechanical Hamiltonian operator, $\hat{H}$, for the given system is:

$$\hat{H} = \frac{\hat{p}^2}{2m} - \hat{q}, \tag{1.20}$$

where $\hat{p}$ and $\hat{q}$ are the momentum and position operators, respectively. Since the Hamiltonian for the system is time-independent the time evolution operator is:

$$\hat{T}(\tau) \equiv e^{-\frac{i}{\hbar}\hat{H}\tau},$$

where the initial time, t_0, is set to zero. For the initial state, $|\alpha\rangle_0$, the time evolution is:

$$\hat{T}(t)\,|\alpha\rangle_0\,.$$

In the position representation the evolution becomes:

$$\langle q|\alpha\rangle_\tau = \int dy\,\langle q|\,\hat{T}(t)\,|y\rangle\,\langle y|\alpha\rangle_0 \tag{1.21}$$

$$= \int dy\,U\,(q,y,\tau)\,\langle y|\alpha\rangle_0. \tag{1.22}$$

The quantity $\langle q|\,\hat{T}(\tau)\,|y\rangle \equiv U\,(q,y,\tau)$ is the quantum mechanical propagator, and is a solution to the time-dependent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 U}{\partial q^2} - qU = i\hbar\frac{\partial U}{\partial \tau}, \tag{1.23}$$

here the Hamiltonian (1.20) is in the configuration representation. Note that there are two conditions the quantum mechanical propagator satisfies:

$$\lim_{\tau \to 0} U\,(q,y,\tau) = \lim_{\tau \to 0} \langle q|\,\hat{T}(\tau)\,|y\rangle \equiv \delta(q-y), \tag{1.24}$$

$$U(0,y,t) = 0. \tag{1.25}$$

The initial condition is specific to the configuration representation, while the boundary condition is general and due to the impenetrable barrier at the origin. The WKB ansatz requires assuming the propagator for times $\tau > 0$ will be:

$$U(q,\tau) \sim A(q,\tau)\,e^{\frac{i}{\hbar}S(q,\tau)}. \tag{1.26}$$

Inserting this representation into equation (1.23) and making a formal series expansion in powers of $\hbar$ yields, to order $\hbar^0$:

$$\frac{1}{2m}\left(\frac{\partial S(q,\tau)}{\partial q}\right)^2 + V(q) + \frac{\partial S(q,\tau)}{\partial \tau} = 0, \tag{1.27}$$

which is the Hamilton-Jacobi (HJ) equation of classical mechanics [7]. The solution is known as "Hamilton's principal function", or the action. The solution to the HJ equation will admit a family of trajectories, $q(\tau,\alpha)$, where α specifies the initial and final data. For the present problem α is such that $q(t) = x$. Because the Hamiltonian does not depend on the time, the relationship between the action and the energy:

$$E = -\frac{\partial S}{\partial \tau} \tag{1.28}$$

is valid. The main characteristic of the action is its derivative with respect to position:

$$p(q) = \frac{\partial S}{\partial q}. \tag{1.29}$$

A similar relationship for the case where the trajectory is given initial momentum is:

$$\frac{\partial S}{\partial p} = y. \tag{1.30}$$

This paper will use the evaluation of equations (1.29) and (1.28) for $\tau = t$, and (1.30) check the validity of the actions in the following chapters:

$$\frac{\partial S}{\partial x} = p(t), \tag{1.31}$$

$$\frac{\partial S}{\partial t} = -E, \tag{1.32}$$

$$\frac{\partial S}{\partial p} = y. \tag{1.33}$$

The total time derivative of the action is the Lagrangian of the system, $L(\dot{q}, q, \tau)$. Therefore, if the trajectories are already known the construction of the action is the

indefinite time integral of the system Lagrangian with a constant of integration to satisfy (1.31)-(1.33):

$$S(q, \tau) = \int L(\dot{q}, q, \tau) \, d\tau + C. \tag{1.34}$$

For trajectories interacting with the ceiling the separate indefinite time integrals of the Lagrangians corresponding to each trajectory before and after the bounce yields the action up to a constant:

$$S_b(q, \tau) = \int L(\dot{q}_1, q_1, \tau) d\tau + \int L(\dot{q}_2, q_2, \tau) \, d\tau + C. \tag{1.35}$$

Again, the constant of integration ensures the validity of equations (1.31)-(1.33).

To the order $\hbar^1$ substitution of the WKB ansatz into the time-dependent Schrödinger equation yields:

$$\partial_q [A(q, \tau) \, p(\tau)] + p(\tau) \, \partial_q A(q, \tau) = -\partial_\tau A(q, \tau), \tag{1.36}$$

again equation (1.29) defines $p(\tau)$. Defining the density function $\rho(q, \tau) \equiv |A(q, \tau)|^2$, the amplitude equation becomes [5]:

$$\partial_\tau \rho(q, \tau) = -\partial_q \{\rho(q, \tau) \, v(\tau)\}, \tag{1.37}$$

where $v(\tau) = \frac{p(\tau)}{m} = 2 \, p(\tau)$. The quantity $\rho(q, \tau)$ has the interpretation of a density of classical particles in the N-dimensional subspace spanned by q of the 2N dimensional phase-space such that the number of particles between q and $q + dq$ is $\rho(q, \tau) \, dq$. Note that the subspace describing the density is not necessarily position as a function of momentum, but is any set of canonical variables. The total number of particles at time τ in the subspace spanned by q is:

$$N(\tau) = \int dq \, \rho(q, \tau),$$

which remains constant for all values of time. Therefore, the Jacobian representing the change in canonical coordinates from $q_1(\tau_1)$ to $q_2(\tau_2)$ governs the evolution of the density function:

$$\rho(q_2, \tau_2) = \rho(q_1, \tau_1) \left| \frac{\partial q_1}{\partial q_2} \right|. \tag{1.38}$$

Therefore, the transformation of the amplitude function is in general:

$$A(\mathbf{r}) = A(\mathbf{u}) \left| \mathbf{J}(\mathbf{r}, \mathbf{u}) \right|^{\frac{1}{2}}, \tag{1.39}$$

here $\mathbf{u}$ represents the initial representation describing the the density function and $\mathbf{r}$ is the final. The determination of the initial amplitude, $A(\mathbf{u})$, is such that the WKB propagator agrees with the correct analytic propagator initially and at the ceiling, equations (1.24) and (1.25) respectively.

Therefore, the general form of the WKB propagator with initial data y and final data (x, t) to $\mathcal{O}(\hbar)$ is:

$$K(x, y, t) = A(\mathbf{u}) \left| \mathbf{J}(\mathbf{r}, \mathbf{u}) \right|^{\frac{1}{2}} e^{\frac{i}{\hbar} S(x, y, t)}. \tag{1.40}$$

Here the explicit dependence of the action on the initial parameter y reveals the propagator acts on states initially in configuration space. However, since the initial position is a parameter the Jacobian in equation (1.39) will diverge for all final data if the initial density of classical particles is given in the position representation of phase space. To avoid this divergence the characterization of the initial density is in the momentum subspace, and the final representation is in position.

The relationship between the quantum mechanical propagators with initial position data, $\langle x | \hat{T}(\tau) | y \rangle = U(q, y, \tau)$, and that with initial momentum data, $\langle x | \hat{T}(\tau) | p \rangle =$

$\hat{U}(q, p, \tau)$ is:

$$
\begin{aligned}
\langle q|\alpha\rangle_\tau &= \int_{-\infty}^{\infty} dy \, \langle x| \hat{T}(t) |y\rangle \, \langle y|\alpha\rangle_0 \\
&= \int_{-\infty}^{\infty} dp \, \langle x| \hat{T}(t) |p\rangle \, \langle p|\alpha\rangle_0,
\end{aligned} \tag{1.41}
$$

where $\langle p|\alpha\rangle_0$ is the Fourier transform of the initial state vector:

$$
\begin{aligned}
\langle p|\alpha\rangle_0 &= \int_{-\infty}^{\infty} dy \, \langle p|y\rangle \langle y|\alpha\rangle_0 \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dy \, e^{-\frac{i}{\hbar}py} \langle y|\alpha\rangle_0.
\end{aligned}
$$

This relationship is valid for the WKB approximations also. However, the constraints on the initial data due to the classical considerations will not allow the integration ranges in (1.21) and (1.41) to cover all possible values. If the regions the classical constraints do not allow integration over correspond to regions where the quantum mechanical propagator oscillates violently or has high damping then the approximation should be accurate. The construction of the WKB propagator corresponding to trajectories given initial momentum data is identical to the initial position construction. Inconsistencies arise from the difference in the constraints on the initial data and the form of the action. In contrast to equation (1.24), the initial form of the propagator with initial momentum data is:

$$
\lim_{\tau \to 0} U(x, p, \tau) = \lim_{\tau \to 0} \left\langle x \left| \hat{T}(\tau) \right| p \right\rangle \equiv \frac{e^{\frac{i}{\hbar}xp}}{\sqrt{2\pi\hbar}}. \tag{1.42}
$$

And it is this condition which the initial amplitudes must generate for the initial momentum case, as well as equation (1.25).

CHAPTER II

TRAJECTORIES WITH GIVEN INITIAL POSITION DATA

Throughout this chapter the denotation of initial, (p, t_0), and final data, (x, t), is:

$$\mathbf{d}_y \equiv [(p, 0), (x, t)]$$

$$\mathbf{b}_y \equiv [(p, 0), (0, b_y)]$$

$$\mathbf{r}_y \equiv [(-p - b_y, b_y), (x, t)],$$

here b_y denotes the time of bounce for trajectories given initial position data.

Using equation (1.10), the general trajectory and momentum connecting the initial data (y, t_0) to the final data (x, t) for the linear potential are:

$$q(\tau; \mathbf{x}_y) = (\tau - t_0)^2 + (\tau - t_0)\left[\frac{x - y}{t - t_0} - (t - t_0)\right] + y \tag{2.1}$$

$$p(\tau; \mathbf{x}_y) = (\tau - t_0) + \frac{1}{2}\left[\frac{x - y}{t - t_0} - (t - t_0)\right]. \tag{2.2}$$

For the direct path $t_0 \to 0$ in $\mathbf{x}_y$, and the trajectory and momentum are:

$$q(\tau; \mathbf{d}_y) = \tau^2 + \tau\left[\frac{x - y}{t} - t\right] + y \tag{2.3}$$

$$p(\tau; \mathbf{d}_y) = \tau + \frac{1}{2}\left(\frac{x - y}{t} - t\right). \tag{2.4}$$

Note that equation (2.4) implies that the trajectory with initial momentum equal to zero will have an initial position given by:

$$\tilde{y} = x - t^2, \tag{2.5}$$

in agreement with the arguments of the introduction.

The Hamiltonian of the non-bounce trajectories is given by:

$$H_{y,d} = p(t)^2 - x = \frac{1}{4t^2}\left(y^2 - 2y\left(t^2 + x\right) + (x - t^2)^2\right), \tag{2.6}$$

and the constraints on the energy being positive or negative are thus:

$$H_{y,d} \;>\; 0: \; y \in \left(-\infty, \left(t - \sqrt{x}\right)^2\right) \cup \left(\left(t + \sqrt{x}\right)^2, \infty\right) \tag{2.7}$$

$$H_{y,d} \;=\; 0: \; y = \left(t \pm \sqrt{x}\right)^2 \tag{2.8}$$

$$H_{y,d} \;<\; 0: \; y \in \left(\left(t - \sqrt{x}\right)^2, \left(t + \sqrt{x}\right)^2\right). \tag{2.9}$$

Using equations (2.2) and (2.1) the trajectories and momenta for the bounce paths are:

$$q(\tau; \mathbf{b}_y) \;=\; \tau^2 - \tau\left(b + \frac{y}{b}\right) + y \tag{2.10}$$

$$q(\tau; \mathbf{r}_y) \;=\; \left(\tau^2 - t^2\right) + \frac{\tau - t}{b - t}\left(-\left(b^2 - t^2\right) - x\right) + x \tag{2.11}$$

$$p(\tau; \mathbf{b}_y) \;=\; \tau - \left(\frac{y}{2b} + \frac{b}{2}\right) \tag{2.12}$$

$$p(\tau; \mathbf{r}_y) \;=\; \tau - \frac{1}{2}\left(\frac{x}{b - t} + (b + t)\right), \tag{2.13}$$

and the corresponding Hamiltonian is:

$$H_{y,b} = p_1(b)^2 = \frac{(b^2 - y)^2}{4b^2}. \tag{2.14}$$

Using equations (1.17) and (2.4), the time at which the particle will turn-around, n_y, is:

$$n_y = -p_0 \;=\; -\left(\frac{x - y}{2t} - \frac{t}{2}\right) \Rightarrow$$

$$n_y \;=\; \frac{1}{2}\left(\frac{y - x}{t} + t\right). \tag{2.15}$$

A. Trajectories of Type (1)

Since the potential drives the particle away from the ceiling, the final momentum of a particle initially moving away from the ceiling will also be positive, therefore the only constraint to impose on trajectories of type (1) is:

$$p\left(0\right) > 0 \Rightarrow y < x - t^2 = \tilde{y}, \tag{2.16}$$

which describes the fact that as the initial momentum of the particle is positively increased from zero the initial position will be pushed away from the limiting value, $\tilde{y}$. However, as noted in the introduction, in order to ensure that $y > 0$, it must be that $x > t^2$. Therefore the correct constraint is:

$$x > t^2 : \ \ y < x - t^2. \tag{2.17}$$

Note that $t^2 \Rightarrow \frac{\alpha t^2}{2m}$, which is the displacement of a particle with zero initial velocity. Therefore, requiring $x - y > t^2$ implies there must be an initial positive momentum to alow the particle to reach the final destination within time t. Therefore, the conflict arising which constrains the the final data is that for given (x, t) as the initial momentum is increased the initial position must be set closer to the ceiling, and the limiting case is $y = 0 \Rightarrow x = t^2$.

The energy of the direct trajectory may be negative or positive. From equations (2.7) and (2.9) the energy of the direct trajectories may be divided into:

$$
\begin{aligned}
E > 0 : \ \ y \ &\in \ \left(0, \left(\sqrt{x} - t\right)^2\right) \\
E < 0 : \ \ y \ &\in \ \left(\left(\sqrt{x} - t\right)^2, x - t^2\right).
\end{aligned}
$$

B. Trajectories of Type (2)

If a trajectory initially and finally moves toward the ceiling then the momentum gained during flight, t, must be less than the momentum to turn the particle around, $t < n_y$, using equation (2.15) reveals:

$$y > x + t^2. \tag{2.18}$$

Since the particle will not turn around it will travel a total distance $\Delta = y - x$. Therefore equation (2.18) states that the total distance for the direct trajectory is greater than the minimum turning trajectory distance, implying the necessity of an initial negative momentum, cf. (1.18). Unlike (2.17) there is no constraint on the relationship between the final data (x, t). This is because for given final data (x, t), as the initial momentum increases negatively the initial position will move away from the non-physical region, not towards. Therefore, the positivity requirement on x and t is enough to ensure that the trajectory will not pass into the forbidden region, for initial negative momentum.

Finally, note that the energy may again be positive or negative depending on the relationship between y and (x, t):

$$E < 0 : \quad y \in \left(x + t^2, \left(\sqrt{x} + t \right)^2 \right)$$
$$E > 0 : \quad y \in \left(\left(\sqrt{x} + t \right)^2, \infty \right)$$
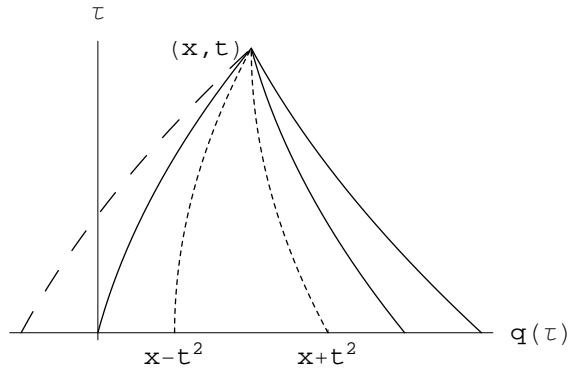
Fig. 5. Plot of direct trajectories for final data (x, t). The dotted line emanating from $x - t^2$ is the critical curve for trajectories of type (1), all other allowable paths lie to the left of the critical curve and to the right of the ceiling. The dashed line represents a forbidden trajectory. The dotted line emanating from $x + t^2$ is the critical curve for type (2) trajectories, all allowable paths lie to the right of this trajectory. Note that in the region $y \in (x - t^2, x + t^2)$ no direct trajectories exist, this is where the type (3) trajectories will be prevalent.

C. Trajectories of Type (3)

One constraint governing trajectories of type (3) is that the position at which the particle turns around must be in the physical region :

$$q(n) > 0. \tag{2.19}$$

Since the energy is time independent, $E = -q(n)$, therefore equation (2.19) prohibits the energy from being positive. The constraints on the initial position to ensure the energy is negative are given by equation (2.9):

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

However, there exist two other constraints on the trajectory:

$$p(0) \ < \ 0, \tag{2.20}$$

$$t \ > \ n_y. \tag{2.21}$$

Using (2.4) and (2.15) these constraints collectively imply:

$$y \ \in \ \left(x - t^2, x + t^2\right) \Rightarrow$$
$$y \ \in \ \left(\left(\sqrt{x} - t\right)\left(\sqrt{x} + t\right), \left(t + \sqrt{x}\right)^2 - 2t\sqrt{x}\right). \tag{2.22}$$

Comparing (2.9) and (2.22), the upper bound on the initial position is:

$$y < x + t^2,$$

and the two possible lower bounds on y are:

$$\left(\sqrt{x} - t\right)\left(\sqrt{x} + t\right), \tag{2.23}$$
$$\left(\sqrt{x} - t\right)\left(\sqrt{x} - t\right). \tag{2.24}$$

If $\sqrt{x} < t$ then Eq.(2.23) is negative and hence the lower bound for y is Eq.(2.24). For $\sqrt{x} > t$ both bounds will be positive, but since $\sqrt{x} - t < \sqrt{x} + t$, Eq.(2.24) is the proper lower bound. Since whether $\sqrt{x}$ is greater or less than t does not affect the upper bound, the constraints on the initial position for a trajectory which turns around are:

$$\sqrt{x} < t : (\sqrt{x} - t)^2 < y < x + t^2 \tag{2.25}$$
$$\sqrt{x} > t : \quad x - t^2 < y < x + t^2. \tag{2.26}$$

Figure (5) gives a graphical representation of the direct trajectories.

D.   Bounce Trajectories

Using equations (2.12) and (2.13) for the requirement that the initial and final momentum be less than and greater than zero, respectively, yields the equations:

$$p(0; \mathbf{b}_y) < 0 \quad \Rightarrow \quad -\frac{1}{2}\left(\frac{y}{b_y} + b_y\right) < 0 \tag{2.27}$$

$$p(t; \mathbf{r}_y) > 0 \quad \Rightarrow \quad \frac{1}{2}\left(\frac{x}{t - b_y} - (t - b_y)\right) > 0 \Rightarrow x > -(t - b)^2. \tag{2.28}$$

Therefore, the constraints of positivity on the parameters (x, y, t) are enough such that the momentum requirements of the trajectories have no implications. Also, equation (2.14) implies that the energy of the bounce trajectory must be positive, with the limiting value of zero. The general constraint on the positivity of the bounce Hamiltonian is thus:

$$H_{y,b} = \frac{1}{4b_y^2}\left(b_y^4 + y^2 - 2b_y^2 y\right) > 0 \Rightarrow \left(b_y^2 - y\right)^2 > 0,$$

therefore the general energy requirement on the trajectory also has no bearing. However the limiting bounce trajectory is identical with the turning point trajectory corresponding to the same energy:

$$\begin{aligned} H_{y,d} &= \frac{1}{4t^2}\left(y^2 - 2y\left(t^2 + x\right) + \left(t^2 - x\right)^2\right) = 0 \Rightarrow \\ y &= \left(t \pm \sqrt{x}\right)^2. \end{aligned}$$

Comparing this result with the inequality in equation (2.25), the correct root is $(t - \sqrt{x})^2$. Therefore on the critical bounce trajectory the relationship between the parameters is:

$$\sqrt{y} + \sqrt{x} = t, \tag{2.29}$$

which agrees with equation (1.19). For given final data, increasing the momentum at the ceiling from zero will require the particle to move to the final position in a time less than that of the critical trajectory, $\sqrt{x}$. Therefore, to not alter the final data the initial position will move away from the ceiling, and hence increase $\sqrt{y}$. The governing constraint on the bounce trajectories is therefore:

$$\sqrt{x} + \sqrt{y} \geq t. \tag{2.30}$$

The ceiling condition for the bounce trajectory, $q_1(b) = -q_2(b)$, yields the equation:

$$f(b) \equiv b^3 + a_2 b^2 + a_1 b + a_0 = 0 \tag{2.31}$$

$$a_2 \equiv -\frac{3}{2}t \tag{2.32}$$

$$a_1 \equiv \frac{t^2}{2} - \frac{1}{2}(x + y) \tag{2.33}$$

$$a_0 \equiv \frac{yt}{2}. \tag{2.34}$$

The polynomial discriminant of the cubic equation, D, is defined as [8]:

$$D \equiv R^2 + Q^3 =$$

$$\frac{t^2}{64}\left((x-y)^2 - \frac{4}{9}(x+y)^2\right) - \left(\frac{t^2}{12}\right)^3 - \left(\frac{1}{6}(x+y)\right)^3 - \frac{t^4}{288}(x+y), \tag{2.35}$$

where the definitions of R and Q are:

$$Q = \frac{3a_1 - a_2^2}{9} = -\frac{t^2}{12} - \frac{1}{6}(x+y) \tag{2.36}$$

$$R = \frac{9a_1 a_2 - 27a_0 - 2a_2^3}{54} = \frac{t}{8}(x - y). \tag{2.37}$$

If $D > 0$ then one root will be real and the other two are complex conjugates, $D = 0$ if all roots are real and at least two are equal, and $D < 0$ for all roots being

real and unequal. From equation (2.35):

$$D(t = 0) \;<\; 0 \tag{2.38}$$

$$\lim_{t \to \infty} D(t) \;=\; -\infty. \tag{2.39}$$

To analyze the discriminant's behavior as $t \to \infty$ let $T \equiv t^2$, then:

$$\frac{dD}{dT} = \frac{1}{64}\left((x-y)^2 - \frac{4}{9}(x+y)^2\right) - \left(\frac{T}{24}\right)^2 - \frac{T}{144}(x+y). \tag{2.40}$$

Therefore, the derivative of the discriminant will tend to $-\infty$ as $t \to \infty$. Setting the above equation to zero reveals the character of the critical points of the polynomial discriminant:

$$T^2 + 4(x+y)T - 9\left((x-y)^2 - \frac{4}{9}(x+y)^2\right) \;=\; 0 \Rightarrow \tag{2.41}$$

$$\pm\sqrt{(x(-2\pm 3) - y(2\pm 3))} \;=\; t.$$

The two negative roots are not physical, therefore the only possible critical points are:

$$t_{c+} = \sqrt{x - 5y}$$

$$t_{c-} = \sqrt{y - 5x}.$$

Since the discriminant is initially less than zero and moves toward $-\infty$, if the initial and final data do not satisfy $x > 5y$ or $y > 5x$ then the derivative of the discriminant will always be negative and hence so will the discriminant. If the final data does satisfy one of the above inequalities then only one of the positive roots will be real. Without loss of generality assume $x > 5y$, therefore the root of equation (2.42) is t_{c+}. Furthermore, equations (2.38) and (2.39) imply that this root must be a maximum for $D(t)$. Therefore, if $D(t_{c+}) < 0$ then the polynomial discriminant will be negative

for all values of t. Using equation (2.35):

$$D(t_{c+}) = \frac{1}{64}\left((x-5y)(x-y)^2 - (x-y)^3\right).$$

Which implies the discriminant will always be negative if:

$$\left((x-5y)(x-y)^2 - (x-y)^3\right) < 0 \Rightarrow$$
$$x - 5y < x - y \Rightarrow$$
$$0 < 4y.$$

Therefore, provided that $y \neq 0$, $D(t) < 0$ for all t and all three roots to equation (2.31) are real and unequal. Similarly, if $y > 5x$ then the requirement that $D(t) < 0$ is $0 < x$, which is in general true except for the special case $x = 0$. The special cases $y = 0$ and $x = 0$ respectively imply that the initial and final positions are at the ceiling, and the time of bounce should respectively be 0 and t.

The maximum and minimum of the cubic equation are:

$$\frac{df\,(b)}{db} = 0 \Rightarrow$$
$$b_{c\pm} = \frac{t}{2} \pm \sqrt{\frac{t^2}{12} + \frac{1}{6}(x+y)},$$

and the point at which the equation changes its concavity is $\frac{t}{2}$. Since $b \rightarrow \pm\infty \Rightarrow f(b) \rightarrow \pm\infty$ the point b_{c-} is where $f(b)$ changes from being concave to convex. Since all three roots must be real one root of $f(b)$ will lie between the two extremum, and the other two must lie outside of the range (cf. figure (6)):

$$r_1 \in (-\infty, b_{c-}) \tag{2.42}$$
$$r_2 \in (b_{c+}, \infty) \tag{2.43}$$
$$r_3 \in (b_{c-}, b_{c+}). \tag{2.44}$$

f (b_y)
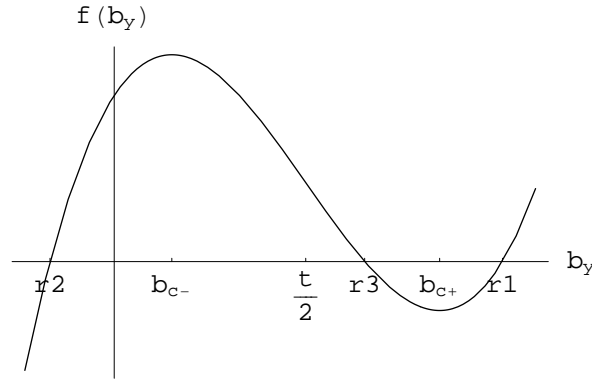
Fig. 6. The cubic equation for the time of bounce. The correct root, r_3, lies in between the maximum and minimum, b_{c+} and b_{c-}, respectively.

Since r_3 is the only root which may equal t and 0, which are the critical values of the bounce time, and the bounce time is a continuous function, r_3 is the correct root for all trajectories. Therefore, if a root of $f(b)$ is found which agrees with the classical trajectories, it will be the correct root for all the trajectories.

For the case where $D < 0$ the cubic roots may be written as:

$$r_1(x,y,t) = \frac{t}{2} + 2\sqrt{-Q(x,y,t)} \cos\left(\frac{\Theta(x,y,t)}{3}\right) \tag{2.45}$$

$$r_2(x,y,t) = \frac{t}{2} + 2\sqrt{-Q(x,y,t)} \cos\left(\frac{\Theta(x,y,t) + 2\pi}{3}\right) \tag{2.46}$$

$$r_3(x,y,t) = \frac{t}{2} + 2\sqrt{-Q(x,y,t)} \cos\left(\frac{\Theta(x,y,t) + 4\pi}{3}\right), \tag{2.47}$$

where the function $\Theta(x,y,t)$ is:

$$\Theta(x,y,t) = \arccos\left(\frac{R(x,y,t)}{\sqrt{-Q(x,y,t)^3}}\right). \tag{2.48}$$

Finally, for a trajectory in which $x = y$, the correct bounce time is $b_y = \frac{t}{2}$, and of the possible roots only (2.47) gives this value. Therefore, by the considerations above $r_3(x,y,t) \equiv b_y$. Note that for the special cases $y = 0$ and $x = 0$, (2.47) gives the

correct values:

$$r_3(x, 0, t) = 0 \tag{2.49}$$

$$r_3(0, y, t) = t. \tag{2.50}$$

Note that to leading order, the limit of the time of bounce as $t \to 0^+$ is:

$$\lim_{t \to 0^+} b_y = \frac{y\,t}{x + y}, \tag{2.51}$$

this equation will be prevalent when considering the asymptotic behavior of the action and amplitude.

The summary of constraints on the initial position are given in Table I. The allowable paths for initial and final data (y, x, t) are deducible from the table by organizing the final data into two categories:

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

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

Note that the direct path $(p_0 < 0)$ belongs to both categories.

Considering category (1), both direct paths and the turning path constrain the initial position into mutually exclusive intervals:

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

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

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

Therefore, for $x \in (t^2, \infty)$ only one of the above paths is possible. However, the region for the bounce trajectories, $y \in ((\sqrt{x} - t)^2, \infty)$, is within each of the above allowable non-bounce regions.

For $x \in (0, t^2)$, the other turning path and the direct path $(p_0 < 0)$ again constrain y into the respective mutually exclusive intervals:

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

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

the bounce interval is also within these intervals.

Therefore, there are at most two allowable trajectories for given initial and final data, the bounce path and one non-bounce. However, if a bounce path does not exist then according to equation (2.30):

$$\sqrt{x} + \sqrt{y} < t$$

$$\Rightarrow y \in (0, (t - \sqrt{x})^2).$$

This region of initial position data is explicitly exclusive from all the possible trajectories except the direct $(p_0 > 0)$ trajectory. However, since the direct $(p_0 > 0)$ trajectory is only valid for $x \in (t^2, \infty)$, the interval of initial data becomes imaginary, $\sqrt{y} < t - \sqrt{x} < 0$, which is physically impossible. In conclusion there will always be either one bounce path and one non-bounce path $\left(\sqrt{y} + \sqrt{x} > t\right)$, or no possible paths $\left(\sqrt{y} + \sqrt{x} < t\right)$, for given initial and final data (y, x, t). Note that in the limiting case, $\sqrt{y} + \sqrt{x} = t$, the bounce path and non-bounce path are identical.

E.   The Classical Action

The complete WKB construction requires the determination of the action of the trajectories and the amplitude function. Using equations (2.1) and (2.2) the general Lagrangian for the initial position formulation is:

$$L\left[q, \dot{q}, \tau\right] \;\; = \;\; p(\tau; \mathbf{x}_y)^2 + q(\tau; \mathbf{x}_y)$$

Table I. Constraints on the initial position with final data. The inequalities were checked using Mathematica.

$x \in$	$y \in$	Trajectory
(t^2, ∞)	$(0, x - t^2)$	Direct, $p_0 > 0$
$(0, \infty)$	$(x + t^2, \infty)$	Direct, $p_0 < 0$
$(0, t^2)$	$\left(\left(\sqrt{x} - t \right)^2, x + t^2 \right)$	Turning
(t^2, ∞)	$(x - t^2, x + t^2)$	Turning
$(0, \infty)$	$\left(\left(t - \sqrt{x} \right)^2, \infty \right)$	Bounce

$$
\begin{aligned}
= \ & 2 \left(\tau - t_0 \right)^2 + 2 \left(\tau - t_0 \right) \left[\frac{x - y}{t - t_0} - (t - t_0) \right] \\
& + \frac{1}{4} \left[\frac{x - y}{t - t_0} - (t - t_0) \right]^2 + y.
\end{aligned}
\tag{2.52}
$$

And using (1.34), the action of the most general trajectory for time $\tau = t$, up to the constant of integration, is:

$$
\begin{aligned}
S_y(t; \mathbf{x}_y) \ = \ & \int^t d\tau \, L \left[q, \dot{q}, \tau \right] + C \\
= \ & \frac{2}{3} (t - t_0)^3 + (t - t_0)^2 \left[\frac{x - y}{t - t_0} - (t - t_0) \right] \\
& + (t - t_0) \left(\frac{1}{4} \left[\frac{x - y}{t - t_0} - (t - t_0) \right]^2 + y \right) + C.
\end{aligned}
\tag{2.53}
$$

The partial derivatives of (2.53) with respect to the final position and time are respectively:

$$
\begin{aligned}
\frac{\partial S_y(\mathbf{x})}{\partial x} \ = \ & (t - t_0) + \frac{1}{2} \left[\frac{x - y}{t - t_0} - (t - t_0) \right] \\
= \ & p(t; \mathbf{x}), \\
\frac{\partial S_y(\mathbf{x})}{\partial t} \ = \ & x + p(0, \mathbf{x})^2 - (t - t_0)^2 + 2(t - t_0) \, p(0; \mathbf{x}) \frac{\partial p(0; \mathbf{x})}{\partial t} \\
= \ & -(t - t_0)^2 - p(0; \mathbf{x})^2 - 2p(0; \mathbf{x})(t - t_0) + x
\end{aligned}
$$

$$= -E.$$

Therefore, equations (1.31)-(1.33) are in agreement with the action if the constant of integration is set to zero:

$$
\begin{aligned}
S_y(t; \mathbf{x}_y) &= \frac{2}{3}(t - t_0)^3 + (t - t_0)^2 \left[\frac{x - y}{t - t_0} - (t - t_0) \right] \\
&\quad + (t - t_0) \left(\frac{1}{4} \left[\frac{x - y}{t - t_0} - (t - t_0) \right]^2 + y \right).
\end{aligned}
\tag{2.54}
$$

The actions for the direct and bounce trajectories are respectively:

$$
\begin{aligned}
S_{dy} &= S_y(t; \mathbf{d}_y) \\
&= \frac{2}{3}t^3 + t^2 \left[\frac{x - y}{t} - t \right] + t \left(\frac{1}{4} \left[\frac{x - y}{t} - t \right]^2 + y \right) \\
S_{by} &= S_y(b_y; \mathbf{b}_y) + S_y(t; \mathbf{r}_y) \\
&= \frac{2}{3} \left(b_y^3 + (t - b_y)^3 \right) + b_y^2 \left[\frac{-y}{t} - b_y \right] + b_y \left(\frac{1}{4} \left[\frac{-y}{t} - b_y \right]^2 + y \right) \\
&\quad + (t - b_y)^2 \left[\frac{x}{t} - (t - b_y) \right] + \frac{(t - b_y)}{4} \left(\frac{x}{t} - (t - b_y) \right)^2
\end{aligned}
\tag{2.55}
$$
$$\tag{2.56}$$

Consideration of the limits of the actions as the time of the trajectory and the final position go to zero (from the positive side) is necessary to ensure the boundary and initial condition of the WKB propagator agree with the quantum mechanical propagator.

Using equation (2.50) for the time of bounce, when the final position is at the ceiling the boundary data becomes:

$$
\mathbf{d}_y \quad \rightarrow \quad [(y, 0), (0, t)]
\tag{2.57}
$$

$$
\mathbf{b}_y \quad \rightarrow \quad [(y, 0), (0, t)]
\tag{2.58}
$$

$$
\mathbf{r}_y \quad \rightarrow \quad [(0, t), (0, t)].
\tag{2.59}
$$

Equation (2.54) reveals that the bounce and direct amplitudes will be equal as the

final data moves toward the ceiling:

$$\lim_{x \to 0^+} S_{by} = S_{dy}. \tag{2.60}$$

Together with the amplitude (see the next section) this condition will ensure that the WKB propagator will vanish for $x = 0$.

The leading order term of the general action in the limit as $t \to t_0^+$ is:

$$\lim_{t \to t_0^+} S_y(t; \mathbf{x}_y) = \frac{(x-y)^2}{4(t-t_0)} + \mathcal{O}(t-t_0). \tag{2.61}$$

Using equation (2.54) and (2.51) for the limit of the bounce time, the limits of the WKB phases as time goes to zero are:

$$\lim_{t \to 0^+} S_{yd} = \frac{(x-y)^2}{4t} + \mathcal{O}(t) \tag{2.62}$$

$$\lim_{t \to 0^+} S_{yb} = \frac{y(x+y)^2}{4xt} + \mathcal{O}(t). \tag{2.63}$$

The WKB phase for the direct path exhibits the correct delta function behavior as $x \to y$. Whereas the bounce phase will create violent oscillations in the WKB propagator in the $t \to 0^+$ limit, with an effective contribution of zero upon integration of an initial wave function.

Note that when considering bounce trajectories the partial derivative operators must take the functional dependence of the time of bounce into account, e.g.:

$$\frac{\partial}{\partial x} \to \frac{\partial}{\partial x} + \frac{\partial b_y}{\partial x} \frac{\partial}{\partial b_y}. \tag{2.64}$$

Therefore, applying a partial derivative operator to the action for the bounce trajectories results in the extra term:

$$\frac{\partial}{\partial b_y} \left[S_y(b_y; \mathbf{b}_y) + S_y(t; \mathbf{r}_y) \right]. \tag{2.65}$$

However, equation (2.54) shows that the partial derivative of the general action with respect to the initial time, t_0, is opposite the derivative with respect to the final time:

$$\frac{\partial S_y(t; \mathbf{x}_y)}{\partial t_0} = -\frac{\partial S_y(t; \mathbf{x}_y)}{\partial t}$$
$$= E.$$

Since b_y is the final time for $S_y(b_y; \mathbf{b}_y)$ and the initial time for $S_y(t; \mathbf{r}_y)$, it follows that equation (2.65) is zero.

F. The Amplitude

Since the initial and final position are parameters for this problem the Jacobian in equation (1.38) is undefined. However, using the momentum representation to initially describe the amplitude implies the Jacobian, $\left|\frac{\partial p(0; \mathbf{x}_y)}{\partial x}\right|$, is valid for trajectories with initial position data:

$$A_f(x, y, t) = A_0(x, y, t) \sqrt{\left|\frac{\partial p(0; \mathbf{x}_y)}{\partial x}\right|}. \tag{2.66}$$

Using equation (2.4), the Jacobian corresponding to the direct amplitude yields:

$$\frac{\partial p(0; \mathbf{d}_y)}{\partial x} = \frac{1}{2t}. \tag{2.67}$$

Requiring the initial form of the WKB propagator to agree with the initial form of the quantum mechanical propagator, $\delta(y - x)$, yields the initial amplitude:

$$\lim_{t \to 0} \frac{A_{d0}}{\sqrt{2t}} e^{iS_d(x,y,t)} = \lim_{t \to 0} \frac{A_{d0}}{\sqrt{2t}} e^{\frac{(y-x)^2}{4it}} = A_{d0}\sqrt{2\pi i}\ \delta(y - x) \Rightarrow$$
$$A_{d0} = \frac{1}{\sqrt{2\pi i}},$$

here equation (2.62) gives the correct form of the direct phase in the $t \to 0^+$ limit. Therefore, the amplitude function for the direct path is given by:

$$A_d(t) = \frac{1}{\sqrt{4\pi i t}}. \tag{2.68}$$

Note that in lieu of equation (2.63), the $t \to 0^+$ limit of the bounce part of the WKB propagator will make no contribution with respect to integration over an initial wave function. This corresponds to the fact that as $t \to 0^+$ the number of possible classical bounce trajectories goes to zero. Therefore the amplitude corresponding to the direct propagator is all that is necessary to ensure the equivalence of the WKB propagator and the exact quantum mechanical form in the $t \to 0^+$ limit.

Using b_y from equation (2.47), and $p_1(0)$ from equation (2.12), the Jacobian corresponding to the action for the bounce case is given by:

$$
\begin{aligned}
\frac{\partial p\left(0; \mathbf{b}_y\right)}{\partial x} &= \left(\frac{y}{2b_y^2} - \frac{1}{2}\right)\frac{\partial b_y}{\partial x} \\
&= \left(\frac{y}{2b_y^2} - \frac{1}{2}\right) \\
&\quad \times \frac{\cos\left(\frac{\Theta + 4\pi}{3}\right)}{6\sqrt{-Q}}\left[1 - \frac{Q}{6\sqrt{-D}}\left(\frac{t}{2} + \frac{R}{Q^4}\right)\tan\left(\frac{\Theta + 4\pi}{3}\right)\right]. \quad (2.69)
\end{aligned}
$$

However, linearizing the classical equations of motion for the potential $V = -|q|$, and then "folding" the negative half of the axis onto the positive half produces a more explicit form of the Jacobian. For the given potential:

$$-\frac{\partial V}{\partial q} = \mathrm{sgn}\,(q) = 2\Theta\,(q) - 1, \tag{2.70}$$

and $\Theta\,(q)$ is the Heavyside step function. Differentiating (2.70) with respect to a parameter, α, yields:

$$\frac{\partial}{\partial\alpha}\left[2\Theta\,(q) - 1\right] = 2\delta\,(q) = 2\frac{\delta\left(\tau - b_y\right)}{|\dot{q}\,(b_y)|}\frac{\partial q}{\partial\alpha}. \tag{2.71}$$

Note that using equation (2.12) along with the fact that $p(b_y) < 0$ for the bounce trajectory moving toward the ceiling:

$$|\dot{q}(b_y)| = \frac{y}{b_y} - b_y. \tag{2.72}$$

Therefore, differentiating Hamilton's equations with respect $\alpha \equiv y$ yields:

$$\frac{d}{d\tau}\frac{\partial p}{\partial y} = 2\frac{\delta(\tau - b_y)}{|\dot{q}(b_y)|}\frac{\partial q}{\partial y} \tag{2.73}$$

$$\frac{d}{d\tau}\frac{\partial q}{\partial y} = 2\frac{\partial p}{\partial y}. \tag{2.74}$$

For the trajectory moving toward the ceiling, $\tau < b_y$, equation (2.73) predicts:

$$\frac{d}{d\tau}\frac{\partial p}{\partial y} = 0,$$

so that $\frac{\partial p}{\partial y}$ is a constant. Therefore, defining $\frac{\partial p}{\partial y}(0) \equiv C$ implies:

$$\frac{\partial p}{\partial y}(\tau) = C \tag{2.75}$$

for $\tau < b_y$. The solution to (2.74) for $\tau < b_y$ is:

$$\frac{\partial q}{\partial y} = 2C\tau + 1, \tag{2.76}$$

since $q(0) = y \Rightarrow \frac{\partial q}{\partial y}(0) = 1$. Integrating (2.73) for $\tau > b_y$, and using equation (2.72) yields:

$$\frac{\partial p}{\partial y} = C + \frac{2}{|\dot{q}(b_y)|}\frac{\partial q}{\partial y}(b_y)$$

$$= \frac{C\left[y + 3b_y^2\right] + 2b_y}{y - b_y^2}. \tag{2.77}$$

And using this result for $\frac{\partial q}{\partial y}$ yields:

$$\frac{\partial q}{\partial y}(\tau) = \frac{\partial q}{\partial y}(b_y) + 2\frac{\partial p}{\partial y}\int_{b_y}^{t} d\tau$$

$$= (2\,C\,b_y + 1) + 2\frac{C\left[y + 3b_y^2\right] + 2b_y}{y - b_y^2}\left(t - b_y\right).$$

Since $q(t) = x$ it follows that $\frac{\partial q}{\partial y}(t) = 0$. Therefore, after algebraic manipulations, the constant $C = \frac{\partial p}{\partial y}(0)$ is:

$$\frac{\partial p}{\partial y}(0) = \frac{1}{2}\frac{5b_y^2 - 4tb_y - y}{\left(y - b_y^2\right)b + (t - b_y)\left(y + 3b_y^2\right)}. \tag{2.78}$$

Finally, using this result in (2.77) and the cubic equation (2.31) to simplify the denominator, the sought after Jacobian is:

$$-\frac{\partial p}{\partial y}(t) = \frac{b_y^2 - y}{2\left[-3tb_y^2 + 2\left(t^2 - x - y\right)b_y + 3yt\right]}, \tag{2.79}$$

The minus sign is accountable for the change in the direction of the momentum due to the "folding" of the negative-half axis over, i.e. creating the ceiling.

The initial amplitude function for the bounce trajectories is chosen such that the WKB propagator vanishes at the ceiling, $U_y(0, y, t) = 0$. From equations (2.63) and (2.62) the phases of the direct and bounce parts of the propagator are identical in this limit. Therefore, the initial amplitude for the bounce case must be such that in the $x \to 0^+$ limit the amplitudes are opposite:

$$\lim_{x \to 0^+} A_{yb}(x, y, t) = -A_{yd}(t) = \frac{-1}{\sqrt{4\pi it}}. \tag{2.80}$$

Using (2.50) for the limit of the bounce time, the Jacobian for the bounce paths becomes:

$$\lim_{x \to 0^+}\left|\frac{b_y^2 - y}{2\left[-3tb_y^2 + 2\left(t^2 - x - y\right)b_y + 3yt\right]}\right|^{\frac{1}{2}} = \frac{1}{\sqrt{2t}}, \tag{2.81}$$

therefore the appropriate initial amplitude is $\frac{-1}{\sqrt{2\pi i}}$:

$$A_{yb} = \frac{-1}{\sqrt{2\pi i}} \left| \frac{b_y^2 - y}{2\left[-3tb_y^2 + 2\left(t^2 - x - y\right)b_y + 3yt\right]} \right|^{\frac{1}{2}}. \tag{2.82}$$

Since the critical curve for the bounce path is identical with the trajectory of type (3) for $E = 0$, the relationship between the initial position and b_y is:

$$y = b_y^2, \tag{2.83}$$

on the critical curve. Therefore, the amplitude for the bounce path will vanish on the critical curve, agreing with classical consideratons.

Putting everything together, the WKB propagators for the direct and bounce cases are respectively:

$$U_{yd}(x, y, t) = \frac{\exp\left[i\left(\frac{2}{3}t^3 + t^2\left[\frac{x-y}{t} - t\right] + t\left(\frac{1}{4}\left[\frac{x-y}{t} - t\right]^2 + y\right)\right)\right]}{\sqrt{4\pi it}}, \tag{2.84}$$

$$U_{yb}(x, y, t) = \frac{-1}{\sqrt{2\pi i}} \left| \frac{b_y^2 - y}{2\left[-3tb_y^2 + 2\left(t^2 - x - y\right)b_y + 3yt\right]} \right|^{\frac{1}{2}}$$

$$\times \exp\left[i\left(\frac{2}{3}b_y^3 + b_y^2\left[\frac{-y}{t} - b_y\right] + b_y\left(\frac{1}{4}\left[\frac{-y}{t} - b_y\right]^2 + y\right)\right)\right]$$

$$\times \exp\left[i\left(\frac{2}{3}(t - b_y)^3 + (t - b_y)^2\left[\frac{x}{t} - (t - b_y)\right]\right)\right]$$

$$\times \exp\left[i\frac{(t - b_y)}{4}\left(\frac{x}{t} - (t - b_y)\right)^2\right]. \tag{2.85}$$

Note that, with the exception of the constraints on the initial position, the propagator for the direct paths is identical with that for the linear potential without a ceiling (1.12).

CHAPTER III

TRAJECTORIES WITH GIVEN INITIAL MOMENTUM DATA

Throughout this chapter the denotation of initial, (p, t_0), and final data, (x, t), is:

$$\mathbf{d}_p \equiv [(p, 0), (x, t)]$$

$$\mathbf{b}_p \equiv [(p, 0), (0, b_p)]$$

$$\mathbf{r}_p \equiv [(-p - b_p, b_p), (x, t)]$$

The general classical path and the corresponding momentum connecting the initial data (p, t_0) with final data (x, t) are:

$$q(\tau; \mathbf{x}_p) = (\tau - t)^2 + 2(\tau - t)(p + t - t_0) + x \tag{3.1}$$

$$p(\tau; \mathbf{x}_p) = (\tau - t_0) + p. \tag{3.2}$$

The general Hamiltonian of the classical system is therefore:

$$H(\tau; \mathbf{x}_p) = (t - t_0 + p)^2 - x. \tag{3.3}$$

The position and momentum for the non-bounce case are:

$$q(\tau; \mathbf{d}_p) = (\tau - t)^2 + 2(\tau - t)(p + t) + x \tag{3.4}$$

$$p(\tau; \mathbf{d}_p) = \tau + p, \tag{3.5}$$

and the Hamiltonian for the direct case is:

$$H_{p,d} = (p + t)^2 - x = p^2 + 2pt + t^2 - x, \tag{3.6}$$

The categories for the energy of the direct trajectories are:

$$H_{p,d} > 0 \quad : \quad p \in \left(-\infty, -\sqrt{x} - t\right) \cup \left(\sqrt{x} - t, \infty\right) \tag{3.7}$$

$$H_{p,d} = 0 \quad : \quad p = \pm\sqrt{x} - t \tag{3.8}$$

$$H_{p,d} < 0 \quad : \quad p \in \left(-\sqrt{x} - t, \sqrt{x} - t\right). \tag{3.9}$$

Using equation (3.1) the bounce paths are:

$$q\left(\tau; \mathbf{b}_p\right) = \left(\tau - b_p\right)^2 + 2\left(\tau - b_p\right)\left(p + b_p\right) \tag{3.10}$$

$$q\left(\tau; \mathbf{r}_p\right) = \left(\tau - t\right)^2 + 2\left(\tau - t\right)\left(t - b_p - 2p\right) + x, \tag{3.11}$$

and the momenta of the bounce trajectories are:

$$p(\tau; \mathbf{b}_p) = \tau + p \tag{3.12}$$

$$p(\tau; \mathbf{r}_p) = \left(\tau - b_p\right) - \left(b_p + p\right). \tag{3.13}$$

The Hamiltonian for the bounce trajectories is thus:

$$H_{p,b} = p(b_p; \mathbf{b}_p)^2 = \left(p + b_p\right)^2. \tag{3.14}$$

Note that the bounce Hamiltonian is always greater than or equal to zero, with equality for $p = -b_p$.

Since all must stay on the positive side of the ceiling, a general constraint on the initial momentum for the non-bounce trajectories is:

$$q(0; \mathbf{d}_p) = -t^2 - 2pt + x \geq 0.$$

Therefore a constraint on type (1) trajectories is:

$$0 \leq p \leq \frac{x}{2t} - \frac{t}{2}, \tag{3.15}$$

and a constraint for type (2) and (3) trajectories is:

$$p < \frac{x}{2t} - \frac{t}{2} < 0. \tag{3.16}$$

A. Trajectories of Type (1)

For the particle to initially move away from the ceiling $p > 0$. Equation (3.15) is the only other constraint on the system, therefore:

$$0 < p \leq \frac{x}{2t} - \frac{t}{2},\tag{3.17}$$

is the constraint on the initial momentum for direct trajectories of type (1). Note that similar to the type (1) trajectory for initial position data $x > t^2$ or else the particle will begin behind the ceiling.

B. Trajectories of Type (2)

Besides the requirement that $p < 0$, and equation (3.16), the particle must also not turn around or enter the forbidden region during flight. Equation (3.5) shows that the turning point of the trajectory will occur at $\tau = -p = |p|$, therefore $t < |p|$. Requiring the particle to not turn around and defining $x > 0$ is enough to ensure that the trajectory will not enter the forbidden region. Since $-t < \frac{x}{2t} - \frac{t}{2}$, the constraint on the initial momentum is:

$$p < -t\tag{3.18}$$

for trajectories of type (2).

Note that equation (3.18) is independent of the relationship between x and t because the requirement $p < 0$ implies the particle will always move toward the ceiling and stop before entering the forbidden region for given final data (x, t) both greater than zero, just as in the initial position case. The necessity of the relationship $p < \frac{x - t^2}{2t}$ is to ensure that the final data does not require the particle to begin behind the ceiling, which is only important when the trajectory is such that the particle will

move away from the ceiling for some part of the path (i.e. trajectories of type (1), and (3)).

C. Trajectories of Type (3)

Using equation (3.6), the energy of the particle at the turning point is:

$$
\begin{aligned}
-q(-p\,;\mathbf{d}_p) &= (p+t)^2 - x \Rightarrow \\
q(n_p;\mathbf{d}_p) &= x - (p+t)^2.
\end{aligned}
\tag{3.19}
$$

Just as the initial position case, a turning point trajectory implies that the energy is less than zero otherwise the turning point is behind the ceiling. Using equation (3.9), a constraint on the initial momentum is:

$$
-\sqrt{x} - t < p < \sqrt{x} - t.
$$

Also, the opposite of equation (3.18) must be true, otherwise the turning point would not have time to occur:

$$
t > |p| \Rightarrow p > -t.
\tag{3.20}
$$

If $\sqrt{x} > t \Rightarrow x > t^2$, then the upper bound in equation (3.9) will be positive. Therefore, the regions corresponding to the momentum of the particle and the energy being less than zero are:

$$
\begin{aligned}
x < t^2 &\;:\; p \in \left(-\sqrt{x} - t, \sqrt{x} - t\right) \\
x > t^2 &\;:\; p \in \left(-\sqrt{x} - t, 0\right).
\end{aligned}
$$

However, equation (3.20) implies that the lower bounds must be replaced by $-t$, therefore the correct constraints on the momentum are:

$$x < t^2 \quad : \quad p \in \left(-t, \sqrt{x} - t\right) \tag{3.21}$$

$$x > t^2 \quad : \quad p \in (-t, 0). \tag{3.22}$$

Again, the relationship between the final data is a consequence of requiring the particle be able to reach the point (x, t) from the physical region. Equations (3.19) and (3.20) reveal that this is congruent with confining the energy of the particle to be less than zero and the initial momentum greater than $-t$ for the turning trajectories.

D. Bounce Trajectories

Equations (3.12) and (3.13) guarantee the validity of (1.11), therefoe the final constraint to impose on the bounce trajectories is the location of the ceiling:

$$q(b_p; \mathbf{r}_p) = 0, \tag{3.23}$$

which corresponds to the quadratic equation:

$$b_p^2 + b_p \left(\frac{2}{3}p - \frac{4}{3}t\right) + \frac{1}{3}\left(t^2 - 2pt - x\right) = 0 \Rightarrow$$
$$b_p = \frac{1}{3}\left(2t - p \pm \sqrt{(p+t)^2 + 3x}\right).$$

Requiring the time of bounce to be less than the trajectory time and the initial momentum to be less than zero yields,

$$b_p \leq t \Rightarrow \tag{3.24}$$
$$(|p| - t) \pm \sqrt{(|p| - t)^2 + 3x} \leq 0.$$

Therefore the correct bounce time is:

$$b_p = \frac{1}{3}\left(2t - p - \sqrt{(p+t)^2 + 3x}\right). \qquad (3.25)$$

Constraining the initial position of the trajectory to be in the classical region implies:

$$q(0; \mathbf{b}_p) > 0 \Rightarrow$$

$$0 < b_p < -2p.$$

However, the "critical" trajectory for the bounce path is when the initial momentum is equal to the time of bounce, corresponding to the particle just grazing the ceiling. All other initial momentum must be greater, in magnitude, than the time of bounce:

$$0 < b_p < -p < -2p. \qquad (3.26)$$

Therefore the constraint due to the critical trajectory is stronger than that due to initially confining the particle in the classical region. The initial momentum corresponding to a bounce time equal to zero is the solution to:

$$2t - p - \sqrt{(t+p)^2 + 3x} = 0 \Rightarrow$$
$$\frac{t^2 - x}{2t} = p, \qquad (3.27)$$

and the intersection of the bounce time with the line $-p$ is a solution to the equation:

$$2t + 2p - \sqrt{(t+p)^2 + 3x} = 0 \Rightarrow$$
$$-t \pm \sqrt{x} = p. \qquad (3.28)$$

However, for $x > 0$ any physical solutions must be such that $t + p > 0$, otherwise the above solutions will be imaginary. Using this constraint implies the only real solution
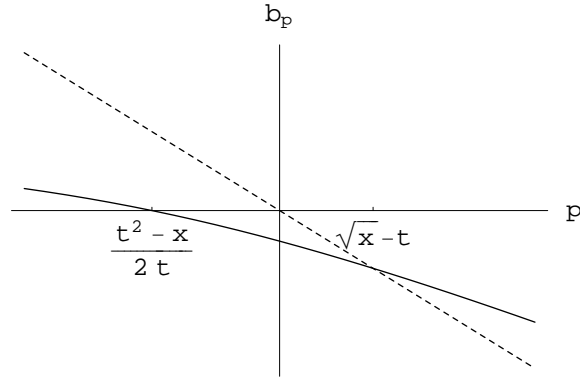
Fig. 7. The bounce time (solid line) and $-p$ (dashed line) for $x > t^2$. The allowable region of initial momentum lies to the left of $\frac{t^2-x}{2t}$, where b_p becomes positive. Note that b_p crosses $-p$ only once.

to the above equation is:

$$p = \sqrt{x} - t. \tag{3.29}$$

Therefore, using equations (3.27) and (3.29), if $x > t^2$ the time of bounce will pass $-p$ for momentum greater than zero and the time of bounce will be greater than zero for negative initial momentum, cf. figure (7). For $x < t^2$ the passage will occur for negative initial momentum and the bounce time will be zero for an initial positive momentum, cf. figure (8). The constraints to impose on the initial momentum such that equation (3.26) holds are thus:

$$x < t^2 : \quad p < \sqrt{x} - t \tag{3.30}$$

$$x > t^2 : \quad p < \frac{t^2 - x}{2t}. \tag{3.31}$$

Note that in lieu of equation (3.30), in the $x \to 0^+$ limit the magnitude of the initial momentum must be greater than the time of the trajectory. Therefore, the
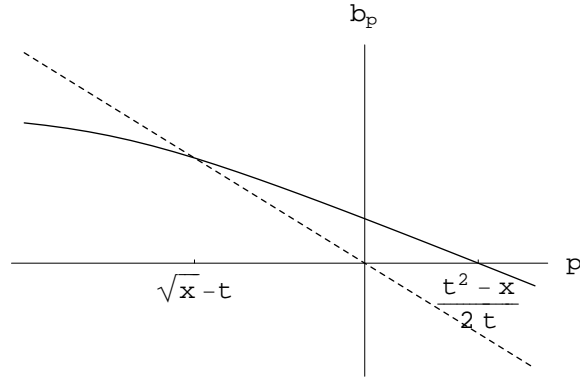
Fig. 8. The bounce time (solid line) and $-p$ (dashed line) for $x < t^2$. The allowable region of initial momentum lies to the left of $\sqrt{x} - t$, where b_p becomes less than $-p$. Note that b_p crosses $-p$ only once.

bounce time becomes:

$$\lim_{x \to 0^+} b_p \quad \to \quad \frac{1}{3}\left(2t - p - |p + t|\right) \Rightarrow$$

$$\lim_{x \to 0^+} b_p \quad = \quad t, \tag{3.32}$$

since $|p + t| = -(p + t)$ in the limit $x \to 0^+$. Also, using equation (3.31) in the limit $t \to 0^+$ the initial momentum goes to $-\infty$. Therefore, in the $t \to 0^+$ limit the bounce time becomes:

$$\lim_{t \to 0^+} b_p \quad \to \quad \lim_{p \to -\infty} \frac{1}{3}\left(-p - \sqrt{p^2 + 3x}\right) = \lim_{p \to -\infty} \frac{p}{3}\left(\sqrt{1 + \frac{3x}{p^2}} - 1\right) \Rightarrow$$

$$\lim_{t \to 0^+} b_p \quad = \quad \mathcal{O}\left(\frac{1}{p^2}\right) \to 0, \tag{3.33}$$

which is valid for non-zero final position and states that as the trajectory time goes to zero the "number" of classical paths able to bounce off the ceiling will also go to zero.

The summary of constraints on the initial momentum for given final data (x, t) is in Table II. There are vivid differences between the allowable paths for given data

(p, x, t) and those for the previous (y, x, t) case. Again, by organizing the constraints into the two classifications $x \in (0, t^2)$ and $x \in (t^2, \infty)$, the allowable trajectories become apparent. Note that the direct $(p < 0)$ trajectory belongs to both classifications just as in the (y, x, t) case.

There are four trajectories corresponding to the $x \in (t^2, \infty)$ case: both direct trajectories, a turning and a bounce. The turning $(p > 0)$ regime is exclusive from the regimes of the other three trajectories. Correspondingly, if the initial momentum is positive only the direct $(p > 0)$ trajectory is allowable. For $p < 0$, further analysis requires to break the region of possible final position into the regions:

- $x \in (t^2, 3t^2)$

- $x \in (3t^2, \infty)$.

For the first region of final data, the direct and turning regions are mutually exclusive, while the bounce region is part of both. Whereas for the second interval of final position the direct and bounce regions are exclusive from the turning region yet the direct region contains the bounce. Therefore, depending on whether $x \in (t^2, 3t^2)$ or $x \in (3t^2, \infty)$ the allowable trajectories for $p < 0$ are: a bounce path and either the direct $(p < 0)$ or the turning; or the bounce and direct $(p < 0)$ or turning, respectively. Whereas for $p > 0$ the only type of trajectory is the direct $(p > 0)$.

For $x \in (0, t^2)$ there are no paths corresponding to positive initial momentum. The intervals corresponding to the direct and the turning trajectories are exclusive and are subsets of the bounce region. Therefore two paths are always possible for $x \in (0, t^2)$, one will always be a bounce, and the other is either the direct $(p < 0)$ or the turning trajectory. Note that this is in contrast to the region $x \in (t^2, \infty)$ where there is a possibility of only one allowable path.

Finally, in comparison with the allowable paths given initial position the major

Table II. Constraints on the initial momentum given the final data. The inequalities
were checked using Mathematica.

$x \in$	$p \in$	Trajectory
(t^2, ∞)	$\left(0, \frac{x-t^2}{2t}\right)$	Direct, $p > 0$
$(0, \infty)$	$(-\infty, -t)$	Direct, $p < 0$
$(0, t^2)$	$(-t, \sqrt{x} - t)$	Turning
(t^2, ∞)	$(-t, 0)$	Turning
$(0, t^2)$	$(-\infty, \sqrt{x} - t)$	Bounce
(t^2, ∞)	$\left(-\infty, \frac{t^2-x}{2t}\right)$	Bounce

difference is that there are regions for (p, x, t) data where only one path may exist, whereas if paths are allowable for (y, x, t) data, i.e. the data satisfies equation (2.30), then there will always be two distinct trajectories.

E.   The Classical Action

Using equations (3.1) and (3.2), the classical Lagrangian for the general initial and final data is:

$$L_p(\tau; \mathbf{x}_p) = (\tau - t_0 + p)^2 + (\tau - t)^2 + 2(\tau - t)(p + t - t_0) + x.$$

Using (1.34), the general action for $\tau = t$ and arbitrary initial and final data, $\mathbf{x}_p$, up to the constant of integration is:

$$S_p(\mathbf{x}_p) = -\frac{(t - t_0)^3}{3} + (t - t_0)\left(x + p^2\right) + S_0. \tag{3.34}$$

The following partial derivatives of the general action will again prove useful in determining the appropriate initial condition:

$$\frac{\partial S_p}{\partial t}(\mathbf{x}_p) = -(t - t_0)^2 + \left(p^2 + x\right) \tag{3.35}$$

$$\frac{\partial S_p}{\partial t_0}(\mathbf{x}_P) = (t - t_0)^2 - \left(p^2 + x\right) = -\frac{\partial S_p}{\partial t} \tag{3.36}$$

$$\frac{\partial S_p}{\partial x}(\mathbf{x}_p) = (t - t_0). \tag{3.37}$$

Using the derivatives of the general initial position, $q(t_0; \mathbf{x}_p)$, from equation (3.1):

$$\frac{\partial q}{\partial t}(t_0; \mathbf{x}_p) = -2(p + t - t_0) \tag{3.38}$$

$$\frac{\partial q}{\partial x}(t_0; \mathbf{x}_p) = 1, \tag{3.39}$$

the correct initial action satisfying equations (1.31) - (1.33) is therefore $S_0 = p(t_0; \mathbf{x}_p)\, q(t_0; \mathbf{x}_p) = p\, q(t_0; \mathbf{x}_p)$:

$$\frac{\partial}{\partial t}(S + S_0) = -(t - t_0)^2 + \left(p^2 + x\right) - 2p(p + t - t_0) = -H(\mathbf{x}_p)$$

$$\frac{\partial}{\partial x}(S + S_0) = (t - t_0) + p = p(t; \mathbf{x}_p)$$

$$\frac{\partial}{\partial p}(S + S_0) = 2p(t - t_0) - 2p(t - t_0) + q(t_0) = q(t_0; \mathbf{x}_p).$$

Note that the terms resulting from the differentiation of b_p contribute to the consistency of $(1.31) - (1.33)$, in contrast to the initial position formulation where the terms cancel each other. Therefore, the actions for the direct and bounce cases are, respectively:

$$\begin{aligned}
S_{pd} &= S_p(\mathbf{d}_p) + p\, q(0; \mathbf{d}_p) \\
&= -\frac{t^3}{3} + (p + t)(x - p\, t) \tag{3.40} \\
S_{pb} &= S_p(\mathbf{b}_p) + S_p(\mathbf{r}_p) + p\, q(0; \mathbf{b}_p) \\
&= -\frac{1}{3}\left[b_p^3 + (t - b_p)^3\right] + (t - b_p)\left(x + (p + b_p)^2\right) - b_p p(p + b_p). \tag{3.41}
\end{aligned}$$

Using (3.33), (3.32) for the bounce time and the above equations the $t \to t_0^+$ and $x \to 0^+$ limits for the phases are:

$$\lim_{t \to t_0^+} S_d = p\,x \tag{3.42}$$

$$\lim_{x \to 0^+} S_d = -p\,t(p+t) \tag{3.43}$$

$$\lim_{t \to t_0^+} S_b = 0 \tag{3.44}$$

$$\lim_{x \to 0^+} S_d = -p\,t(p+t). \tag{3.45}$$

Therefore, the direct phase has the correct initial plane wave form of the correct propagator in the $t \to 0^+$ limit. The bounce phase produces an unnecessary term upon integration over an initial wave function. However, from table II in the $t \to 0^+$ limit the range of initial momentum values goes to $(-\infty, -\infty)$. Therefore the bounce part of the propagator will give vanishing contribution to the initial form of the propagator upon integration over an initial wave function. As with the initial position data case, the $x \to 0^+$ limits will be important when considering the behavior of the WKB propagator at the ceiling.

F.   The Amplitude

The Jacobian corresponding to the amplitude function is $\left| \frac{\partial q(t_0)}{\partial q(t)} \right|$. Using equation (3.1) for the trajectories yields for the direct case:

$$\frac{\partial q(0)}{\partial x} = 1, \tag{3.46}$$

which reveals that the amplitude for the direct case is a constant solely depending on the initial density of particles. This initial density must be in agreement with the the initial form of the quantum propagator in the momentum representation. Equation

(1.42) yields:

$$\lim_{t \to 0} A(x, p, t) = \frac{1}{\sqrt{2\pi}}. \tag{3.47}$$

Therefore, according to equation (1.39) the initial amplitude of the direct propagator is:

$$A_{d0} = \frac{1}{\sqrt{2\pi}}. \tag{3.48}$$

Similarly, using equations (3.10) and (3.11) for the trajectories in the Jacobian for the bounce amplitude yields:

$$\frac{\partial q_1(0)}{\partial x} = \frac{p + b_p}{\sqrt{(p + t)^2 + 3x}}. \tag{3.49}$$

Using equation (3.32) the $x \to 0^+$ limit of the above Jacobian is:

$$\lim_{x \to 0^+} \frac{\partial q_1(0)}{\partial x} = \frac{p + t}{|p + t|} = -1.$$

From equations (3.45) and (3.45) the phases for the direct and bounce paths are equal in the $x \to 0^+$ limit. Therefore the initial amplitude function for the bounce trajectory which satisfies the vanishing requirement at the ceiling is $A_{b0} = \frac{-1}{\sqrt{2\pi}}$, and the correct form of the amplitude function is:

$$A_b = \frac{-1}{\sqrt{2\pi}} \sqrt{\left| \frac{p + b_p}{\sqrt{(p + t)^2 + 3x}} \right|}. \tag{3.50}$$

Recalling that the critical curve for the bounce trajectory is equivalent to the $E = 0$ type (3) trajectory, it is evident that $b_p = n_p = -p$ for the critical trajectory. Hence the amplitude will vanish for the critical path. All other values of b_p are greater than $|p|$. Hence, the numerator of equation (3.50) will be less than zero for bounce paths,

and an equivalent form of the amplitude is:

$$A_{pb} = \frac{i}{\sqrt{2\pi}} \sqrt{\frac{p + b_p}{\sqrt{(p + b_p)^2 + 3x}}}, \tag{3.51}$$

for all bounce trajectories.

To $\mathcal{O}(\hbar)$ the WKB approximation to the quantum propagator is the sum of the sum of the propagators constructed from the bounce and non-bounce paths:

$$U_{pd}(x, p, t) = \frac{1}{\sqrt{2\pi}} \exp\left[i\left(-\frac{t^3}{3} + (x - pt)(p + t)\right)\right] \tag{3.52}$$

$$U_{pb}(x, p, t) = \frac{i}{\sqrt{2\pi}} \sqrt{\frac{p + b_p}{\sqrt{(p + t)^2 + 3x}}} \exp\left[\left(-\frac{1}{3}\left[b_p^3 + (t - b_p)^3\right] - b_p p\,(p + b_p)\right)\right]$$

$$\times \exp\left[\left((t - b_p)\left(x + (p + b_p)^2\right)\right)\right]. \tag{3.53}$$

Note that with the exception of the classical constraints on the initial momentum the propagator corresponding to direct paths is identical to the quantum propagator without a ceiling (1.13).

CHAPTER IV

SUMMARY: COMPARISON OF THE WKB PROPAGATORS

The physical interpretation of the WKB propagator is to approximate the quantum mechanical evolution of an initial wave function by "guiding" it along the corresponding classical paths. The previous chapters display that the consideration of two such evolutions is necessary, i.e. the evolution corresponding to the bounce and non-bounce trajectories. Associating interference patterns in the final WKB wave functions with the interaction of the evolving bounce and non-bounce packets is therefore a logical conclusion. Figure (9) depicts the evolution of an initial Gaussian wave function from an initial time $\tau = 0$ to the final point (x, t). The different curves represent the classical paths in association with the wave packet each carrying a significant weight to the final destination. The stronger influence to the final probability density of initial trajectories emanating from the average value of the initial wave packet, i.e. trajectories with initial data $(\bar{y}, 0)$, is deducible.

This chapter will analyze and compare the propagators of chapters (II) and (III), interpreting the final wave functions in terms of the consequences of the classical evolution of the previous chapters. The comparison of the propagators is made using a gaussian wave packet as the initial quantum state.

A.   The Initial Wave Packet

To simplify the necessary numerical calculations to evaluate the propagators it will be convenient to assume the initial state of the system in position space is a general Gaussian wave packet:

$$\psi\left(y\right) = \left(\frac{2}{\gamma\pi}\right)^{\frac{1}{4}} e^{-\frac{(y-\bar{y})^2}{\gamma} - iy\bar{p}}, \tag{4.1}$$
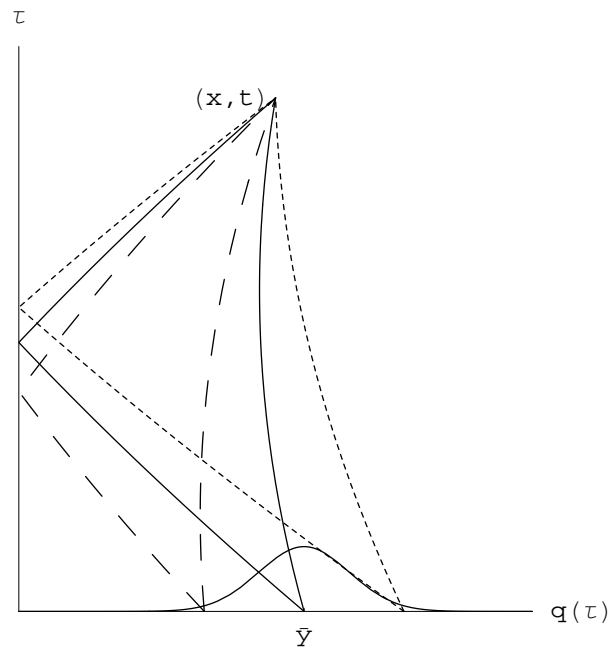
Fig. 9. Plot of semi-classical evolution of the particles composing an initial wave packet to a fixed point (x, t). The solid lines are the classical trajectories for a particle located at the average value of the initial wave packet, and the dashed lines are classical paths associated with trajectories away from the average value.

where y denotes the initial position, the average initial position is $\bar{y}$, and the average initial momentum is $\bar{p}$. The constant γ is associated with the width of the initial wave packet. The initial wave packet in momentum space is the Fourier transform of the initial position space wave packet:

$$\phi\left(p\right) = \left(\frac{\gamma}{2\pi}\right)^{\frac{1}{4}} e^{-\gamma\frac{(p+\bar{p})^2}{4} - i\bar{y}(p+\bar{p})}. \tag{4.2}$$

The choice of the parameters for the wave packets should be chosen so that a negligible amount of the position space wave packet extends into the forbidden region $(y < 0)$.

B. The Propagators Constructed from Non-bounce Paths

From equations (2.84) and (3.52), the propagators constructed from non-bounce trajectories are:

$$U_{yd}\left(x, y, t\right) = \frac{1}{\sqrt{4\pi it}} \exp\left[i\left(\frac{2}{3}t^3 + t^2\left[\frac{x-y}{t} - t\right] + t\left(\frac{1}{4}\left[\frac{x-y}{t} - t\right]^2 + y\right)\right)\right]$$

$$U_{pd}(x, p, t) = \frac{1}{\sqrt{2\pi}} \exp\left[i\left(-\frac{t^3}{3} + t\left(p^2 + x\right) - p\left(t^2 + pt - x\right)\right)\right],$$

and the final wave functions for the initial position and initial momentum formulations are respectively:

$$\begin{aligned}
\Psi_y(x, t) &= \int_{a_y}^{b_y} dy\, \psi(y)\, U_{yd}(x, y, t) \\
&= \left(\frac{2}{\gamma\pi}\right)^{\frac{1}{4}} \frac{\exp\left[-\frac{\bar{y}^2}{\gamma} + i\left(\frac{x^2}{4t} + \frac{xt}{2} - \frac{t^3}{12}\right)\right]}{\sqrt{4\pi it}} \int_{a_y}^{b_y} dy\, e^{-y^2\omega_y + y\lambda_y} \\
&= \left(\frac{2}{\gamma\pi}\right)^{\frac{1}{4}} \frac{\exp\left[-\frac{\bar{y}^2}{\gamma} + \frac{\lambda_y^2}{4\omega_y} + i\left(\frac{x^2}{4t} + \frac{xt}{2} - \frac{t^3}{12}\right)\right]}{\sqrt{4\pi it}} \int_{a_y}^{b_y} dy\, e^{-\left(y\sqrt{\omega_y} - \frac{\lambda_y}{2\sqrt{\omega_y}}\right)^2} \tag{4.3}
\end{aligned}$$

$$\begin{aligned}
\Psi_p(x, t) &= \int_{a_p}^{b_p} dp\, \phi(p)\, U_{yd}(x, y, t) \\
&= \left(\frac{\gamma}{8\pi^3}\right)^{\frac{1}{4}} \exp\left[-\frac{\bar{p}^2\gamma}{4} + i\left(xt - \frac{t^3}{3} - \bar{p}\bar{y}\right)\right] \int_{a_p}^{b_p} dp\, e^{-p^2\omega_p + \lambda_p p}
\end{aligned}$$

$$= \left(\frac{\gamma}{8\pi^3}\right)^{\frac{1}{4}} \exp\left[-\frac{\bar{p}^2\gamma}{4} + \frac{\lambda_p^2}{4\omega_p} + i\left(xt - \frac{t^3}{3} - \bar{p}\bar{y}\right)\right]$$
$$\times \int_{a_p}^{b_p} dp\, e^{-\left(p\sqrt{\omega_p} - \frac{\lambda_p}{2\sqrt{\omega_p}}\right)^2}. \tag{4.4}$$

Here, the limits of integration are consistent with the classical limits given in tables (I) and (II). The functions ω and λ are:

$$\omega_y = \frac{1}{\gamma} - \frac{i}{4t} \tag{4.5}$$

$$\lambda_y = \frac{2\bar{y}}{\gamma} + i\left(\frac{t}{2} - \frac{x}{2t} - \bar{p}\right) \tag{4.6}$$

$$\omega_p = \frac{\gamma}{4} + it \tag{4.7}$$

$$\lambda_p = -\frac{\gamma\bar{p}}{2} + i\left(x - t^2 - \bar{y}\right). \tag{4.8}$$

Since the WKB propagators are equivalent to their exact Quantum Mechanical counterparts, with the exception of the allowable limits of integration, the final wave functions after propagation would be equivalent if not for the WKB limit constraints, in other words the relationship between the WKB propagators in momentum and position space is not the "complete" Fourier transform since the limits of integration do not encompass all possible initial data but only those values which are classically allowable, and the classically allowable regions are not equivalent for the two cases. However, the advantage of using an initial Gaussian wave packet is that if the limits lie outside the "effective" support, $\mathcal{C}_\alpha$, of the initial wave function (i.e. the domain of initial data (position or momentum) such that the initial wave packet is comparable to its maximum, located at $\bar{y}$ or $\bar{p}$), then the extension of the limits in equations (4.3) and (4.4) to $\pm\infty$ is permissible with negligible contribution from the classically forbidden region.

Figure 10 gives a depiction of this behavior for the real parts of the final wave functions. From tables (I) and (II) the classical limits on the initial momentum and
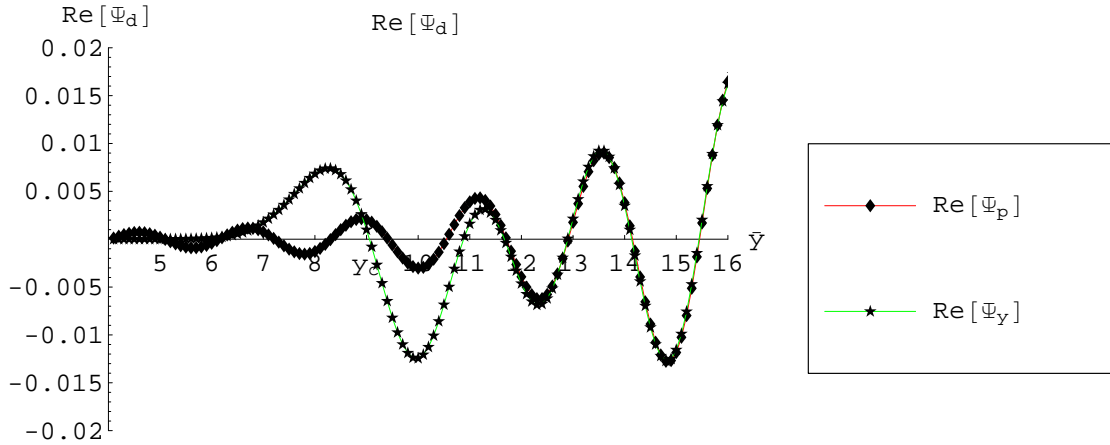
Fig. 10. Equivalence of the evolution of initial wave functions produced by the WKB propagators associated with the classical direct paths. The initial data is such that $\gamma = 2$ and $\bar{p} = -6$. The final data is $(x, t) = (4, 5)$. The average initial position, $\bar{y}$, is varying.

position data are $(-\infty, -3)$ and $(9, \infty)$, respectively. For $\gamma = 2$ the effective supports of the initial wave packets for the momentum and position cases are $(\bar{y} - 2, \bar{y} + 2)$ and $(\bar{p} - 2, \bar{p} + 2)$, respectively (encompassing $\sim 95\%$ of the initial wave packet). Therefore with $\bar{p} = -6$ the final wave function in association with initial momentum data is already approximately exact, and the final wave function with initial position data will agree with the Quantum propagator (and hence the WKB initial momentum propagator) around $\bar{y} \sim 11$. This in in complete agreement with figure 10. Note that the final wave functions in association with bounce paths also begin to agree around $\bar{y} \sim 11$, cf. figure 11.

C.   The Forbidden Region

The WKB propagator for initial position data yields no information for initial wave packets with effective support in the forbidden region, $\mathcal{C}_y \in (0, y_c)$. However, the prop-
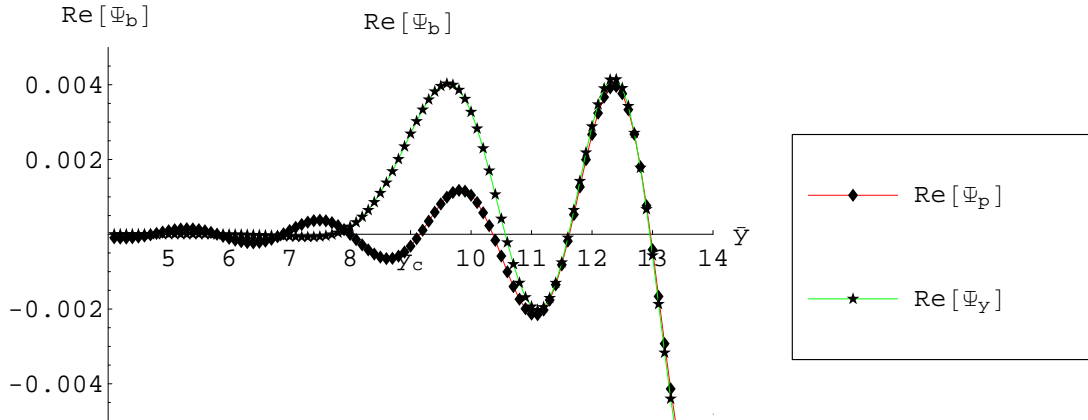
Fig. 11. Equivalence of the evolution of initial wave functions produced by the WKB propagators associated with the classical bounce paths. The initial data is such that $\gamma = 2$ and $\bar{p} = -6$. The final data is $(x, t) = (4, 5)$. The average initial position, $\bar{y}$, is varying.

agator with initial momentum data does yield a contribution to the final probability. The illustration of this phenomenon is in figure 12.

Notice that as the average initial position of the initial wave packet approaches the critical curve, $\bar{y} = y_c = 9$, the probability density begins to spike and then regress with a "Gaussian" form. This behavior is in figure 13.

The phenomenon of the final position and momentum wave functions being in such contrast is explainable in terms of interference in association with the two propagators (direct and bounce) competing. Since on and near the critical curve the bounce part of the initial position propagator vanishes, cf. section(F) , essentially only one wave packet is moving towards the final location, (x, t). In contrast, both components of the initial momentum propagator are present and hence two waves will move toward the final data. Upon interaction, these two waves will interfere resulting in a decrease of probability. Since the analytic evaluation requires all possible paths, the initial momentum propagator is most likely the better approximation for
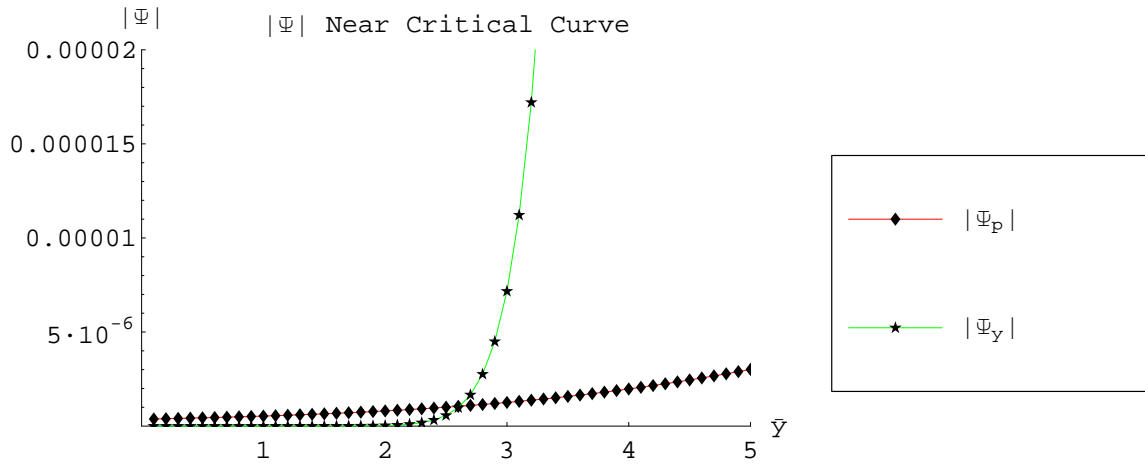
Fig. 12. Probability density for initial wave packets located within the forbidden region of the classical trajectories with initial position. Again $\gamma = 2$, $\bar{p} = -6$, and $(x, t) = (4, 5)$. The average initial position, $\bar{y}$ is varying.
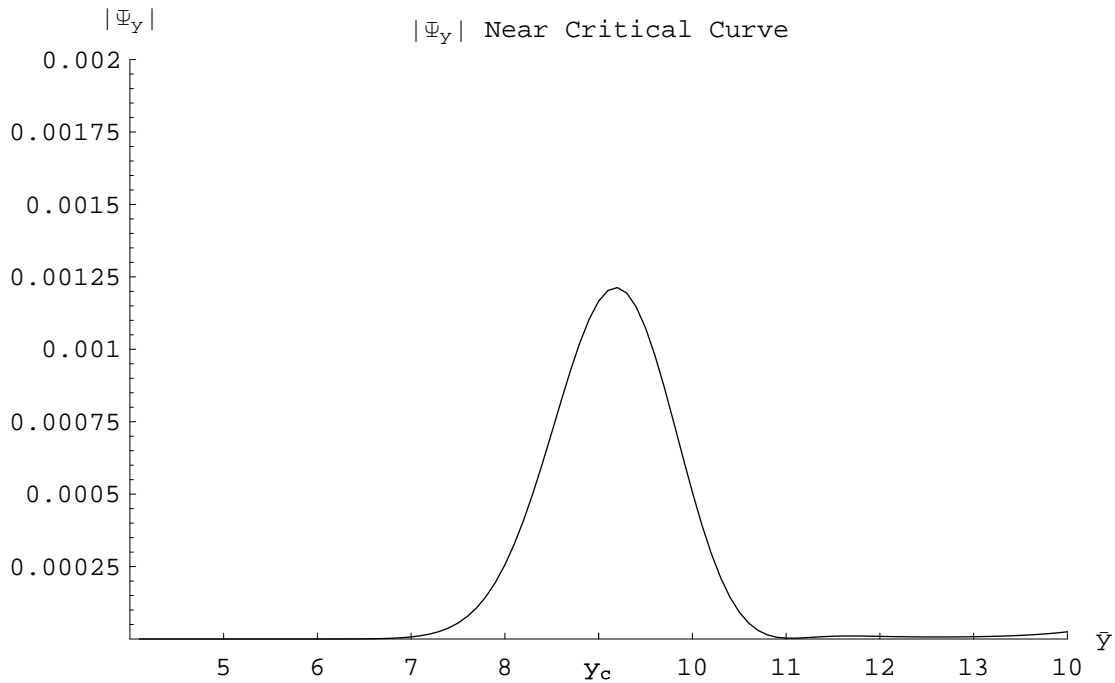

Fig. 13. Probability density for initial position space wave packet with average position located near the critical curve, $y_c = 9$. Again $\gamma = 2$, $\bar{p} = -6$, and $(x, t) = (4, 5)$. The average initial position, $\bar{y}$ is varying.

the scenario.

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VITA

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