A SCHRÖDINGER WAVE MECHANICS FORMALISM FOR THE EIKONAL PROBLEM
AND ITS ASSOCIATED GRADIENT DENSITY COMPUTATION

By

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To my ever-loving and ever-caring Amma and Appa and the person with whom I will be sharing the rest of my life, my beloved fiancée Bhavya.
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By

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Many computational techniques based on classical mechanics exist but surprisingly there isn’t a concomitant borrowing from quantum mechanics. Our work shows an application of the Schrödinger formalism to solve the classical eikonal problem—a nonlinear, first order, partial differential equation of the form $\nabla S = f$, where the forcing function $f(X)$ is a positive valued bounded function and $\nabla$ denotes the gradient operator. Hamiltonian Jacobi based solvers like the fast marching and fast sweeping methods solve for $S$ by the Godunov upwind discretization scheme. In sharp contrast to that, we present a Schrödinger wave mechanics formalism to solve the eikonal equation by recasting it as a limiting case of a quantum wave equation. We show that a solution to the non-linear eikonal equation is obtained in the limit as Planck’s constant $\hbar$ (treated as a free parameter) tends to zero of the solution to the corresponding linear Schrödinger equation.

We begin with, by considering the Euclidean distance function problem, a special case of the eikonal equation where the forcing function is everywhere identically equal to one. We show that the solution to the Schrödinger wave function can be expressed as a discrete convolution between two functions efficiently computable by the Fast Fourier Transforms (FFT). The Euclidean distance function can then be recovered from the exponent of the wave function. Since the wave function is computed for a small but
non-zero $\eta$, the obtained solution is an approximation. We show convergence of our approximate closed form solution for the Euclidean distance function problem to the true solution as $\eta \to 0$ and also bound the error for a given value of $\eta$. Moreover the differentiability of our solution allows us to compute its first and second derivatives in closed form, also computable by a series of convolutions. In order to determine the sign of the distance function (positive inside a close region and negative outside), we compute the winding number in 2D and topological degree in 3D, by explicitly showing that their computations can also be done via convolutions. We show an application of our method by computing the medial axes for a set of 2D silhouettes. A major advantage of our approach over the other classical methods is that, we do not require a spatial discretization of gradient operators as we obtain a closed-form solution for the wave function.

For the general eikonal problem where the forcing can be an arbitrary but positive and bounded function, the Schrödinger equation turns out to be a generalized, screened Poisson equation. Despite being linear, it does not have a closed-form solution. We use a standard perturbation analysis approach to compute the solution which is guaranteed to converge for all positive and bounded forcing functions. The perturbation technique requires a sequence of discrete convolutions which can be performed using the FFT.

Finally using stationary phase approximations we establish a mathematical result relating the density of the gradient(s) of distance function $S$ and the scaled power spectrum of the wave function for small values of $\eta$, when the scalar field $S$ appears as the phase of the wave function. By providing rigorous mathematical proofs, we justify our result for an arbitrary thrice differentiable function in one dimension and for distance transforms in two dimensions. We also furnish anecdotal visual evidences to corroborate our claim. Our result gives a new signature for the distance transforms and potentially serve as its gradient density estimator.
CHAPTER 1
INTRODUCTION

Computational techniques adapted from classical mechanics run the gamut from Lagrangian action principles to Hamilton-Jacobi field equations [22]: witness is the popularity of the fast marching [34, 41] and fast sweeping methods [50] which are essentially fast Hamilton-Jacobi solvers. In sharp contrast, there are very few applications of quantum mechanics-inspired computational methods. Despite the well known fact that most of classical mechanics can be obtained as a limiting case of quantum mechanics (as Planck's constant $\hbar$ tends to zero) [24] and that the linear Schrödinger equations [19, 24] are the quantum counterpart to non-linear Hamilton-Jacobi equations [9], this paucity is somewhat surprising. Rather than speculate on the reasons for this dearth of applications, we wish to point out that in this work, we are primarily interested in exploiting a concrete relationship between the classical, non-linear Hamilton-Jacobi equation [22] and the quantum, linear Schrödinger equation[24]. We feel that focusing more narrowly on this relationship (which will become more obvious as we proceed) is more productive than dwelling on the more mysterious and specifically quantum mechanical issues of i) interpretation of the wave function, ii) role of probabilities and, iii) the problem of measurement [19, 24]. While these issues are certainly important, they do not play any role in this work. The current work demonstrates an applicability of this relationship for a very specific case, namely the eikonal equation and the estimation of its gradient densities.

1.1 Eikonal Equation

The eikonal (from the Greek word $\epsilon\lambda\kappa\nu\sigma\nu$ or “image”) equation is traditionally encountered in the wave and geometric optics literature where the principal concern is the propagation of light rays in an inhomogeneous medium [12]. Its twin roots are in wave propagation theory and in geometric optics. In wave propagation theory, it is obtained when the wave is approximated using the Wentzel–Kramers–Brillouin (WKB)
approximation [35]. In geometric optics, it can be derived from Huygen’s principle [3]. In the present day, the eikonal equation has outgrown its humble optics origins and now finds application in far flung areas such as electromagnetics [35], robot motion path planning [10] and image analysis [28, 33].

The eikonal equation is a nonlinear, first order, partial differential equation [46] of the form

\[ \| \nabla S(X) \| = f(X), \ X \in \Omega \]  

subject to the boundary condition \( S_{\partial \Omega} = U(X) \), where \( \Omega \) is a bounded subset of \( \mathbb{R}^D \). The forcing function \( f(X) \) is a positive valued bounded function and \( \nabla \) denotes the gradient operator. Detailed discussions on the existence and uniqueness of the solution can be found in [16].

The present work concerns with solving the eikonal equation on a discretized spatial grid consisting of \( N \) grid locations from a set of \( K \) point sources \( \{ Y_k \}_{k=1}^K \). Light waves simultaneously emanate from the given point sources and propagate with a velocity of \( \frac{1}{f(X)} \) at the grid location \( X \). The value of \( S \) at a grid point \( X_0 \) \( (S(X_0)) \) corresponds to the time taken by the first light wave (out of the \( K \) light waves) to reach the grid location \( X_0 \).

1.1.1 The Classical Approach

While the eikonal equation is venerable and classical, it is only in the last twenty years that we have seen the advent of numerical methods aimed at solving this problem. To name a few are the pioneering fast marching [34, 41] and fast sweeping [50] methods. Algorithms based on discrete structures such as the well known Dijkstra single source shortest path algorithm [15] can also be adapted to solve this problem. When we seek solutions on a discretized spatial grid with \( N \) points, the complexity of the fast marching method is \( O(N \log N) \) floating-point operations while that of the fast sweeping method is \( O(N) \) and therefore both of these efficient algorithms have seen widespread use since their inception. Recently, the ingenious work of Sapiro et. al. provided an \( O(N) \) implementation of the fast marching method [49]. Fast sweeping
methods have also been extended to the more general static Hamilton-Jacobi equation [27] and also for the eikonal equation on non-regular grids [26, 36]. An Hamiltonian approach to solve the eikonal equation can be found in [42].

The eikonal equation can also be derived from a variational principle [21], namely, Fermat’s principle of least time which states that “Nature always acts by the shortest paths” [4]. The variational problem is denoted by the symbol $L$, called the Lagrangian. The integral of the Lagrangian is called the action of the physical system [22] given by

$$ S^*(X, t) \equiv \int_{t_0}^{t} L dt. $$

(1–2)

For the case when the Lagrangian doesn’t have an explicit dependence on time, the action $S$ can be separated as $S^*(X, t) = S(X) - Et$. The quantity $S$ is called the Hamilton’s characteristic function and $E$ denotes the energy of the system representing the constants of motion [22].

From this variational principle, the classical physics developmental sequence for deriving the eikonal equation proceeds as follows: The first order Hamilton’s equations of motion are derived using a Legendre transformation of the Lagrangian wherein new momentum variables are introduced. Subsequently, a canonical transformation converts the time varying momenta into constants of the motion. The Hamilton-Jacobi equation emerges from the canonical transformation [22]. In the Hamilton-Jacobi formalism specialized to the eikonal problem, the solution to it is actually the Hamilton’s characteristic function $S$. Here we seek a surface such that its increments are proportional to the speed of the light rays $\frac{1}{r(X)}$. This is closely related to Huygen’s principle and thus marks the rapprochement between geometric and wave optics [3]. It is this nexus that drives numerical analysis methods [34, 50] (focused on solving the eikonal equation) to base their solutions around the Hamilton-Jacobi formalism.
1.1.2 The Quantum Mechanical Approach

The importance of Lagrangian $L$ and the action $S^*$ in quantum mechanics was envisioned by Dirac in the early 1930s, when he observed that the short-time propagator [11] (defined in Section 2.2) is the exponential of \(\left\{ \frac{iS^*}{\hbar} \right\}\), where $S^*$ is the classical action. This eventually led Feynman to the invention of quantum-mechanical path integral approach to deriving the Schrödinger wave equation [19].

Since the classical and quantum mechanics are so intimately related [9], it is natural to ask these following questions, namely

- How does the Schrödinger wave equation for the eikonal equation look like?
- Once we derived the corresponding Schrödinger wave equation, how do we solve for the wave function?
- From the computational perspective, how do we efficiently compute it?
- How to retrieve the solution to the original eikonal equation (Equation 1–1) from the wave function?

The present work seeks to answer these questions. Before we proceed, we would like to give a very brief introduction to the Schrödinger wave equation.

Schrödinger wave equation, formulated by the Austrian physicist Erwin Schrödinger in the year 1926, is an equation that describes how the quantum state or the wave function of a physical system evolves in time. It is as central to quantum mechanics as Newton’s laws are to classical mechanics. A quantum state is a most complete description that can be given to a physical system. Solutions to the Schrödinger wave equation can describe quantities ranging from the molecular, subatomic particles to that of the whole universe. The most general form is the time-dependent Schrödinger equation, describing a system that evolves with time. It is written as

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi \quad (1–3)$$

where,
• $\psi(X, t)$ is the wave function with $\psi^* \psi$ carrying a probability interpretation of finding a particle at position $X$ at time $t$.

• $i\hbar \frac{\partial}{\partial t}$ is the energy operator where $\hbar \equiv \frac{h}{2\pi}$ is called the reduced Planck’s constant.

• $\hat{H}$ is the Hamiltonian operator which determines the evolution of the system with time.

If the Hamiltonian operator $\hat{H}$ is independent of time, Equation 1–3 can be factored to obtain time-independent Schrödinger wave equation

$$\hat{H} \phi_n = E_n \phi_n$$

(1–4)

where

• $\phi_n(X)$ is the stationary state wave representing the state of the system that does not change with time.

• $E_n$ is called the energy of the system.

Easy to see that the above system is an eigenfunction system with $\phi_n$ being the eigenfunction of the $\hat{H}$ with an eigenvalue $E_n$. If we know all the eigenfunctions $\phi_n$ of $\hat{H}$, the solution for the time-dependent wave function $\psi(X, t)$ is given by

$$\psi(X, t) = \sum_n c_n e^{-\frac{iE_n t}{\hbar}} \phi_n(X)$$

(1–5)

where $c_n$ are defined by the initial condition

$$\psi_0(X, t_0) = \sum_n c_n e^{-\frac{iE_n t_0}{\hbar}} \phi_n(X)$$

(1–6)

A detailed description of the Schrödinger wave equation, its origin and its properties can be found in [24].

Since the advent of quantum theory, specifically the Schrödinger wave equation, the close relationship between the Schrödinger and Hamilton-Jacobi equations has been intensely studied [9]. Of particular importance here is the quantum to classical transition as $\hbar \to 0$, where the laws of quantum mechanics are assumed to naturally give rise to the laws of classical mechanics. When the time-independent
Hamilton-Jacobi scalar field $S$ is the exponent of the stationary state wave function, specifically $\phi(X) = \exp(-\frac{S(X)}{\hbar})$, and if $\phi(X)$ satisfies the time-independent Schrödinger equation, we show that as $\hbar \to 0$, $S$ satisfies the Hamilton-Jacobi equation. Note that in the above, a nonlinear Hamilton-Jacobi equation is obtained in the limit as $\hbar \to 0$ of a linear Schrödinger equation which is novel from a numerical analysis perspective. Consequently, instead of solving the Hamilton-Jacobi equation, one can solve its Schrödinger counterpart (taking advantage of its linearity), and compute an approximate $S$ for a suitably small value of $\hbar$. This computational procedure is approximately equivalent to solving the original Hamilton-Jacobi equation.

Surprisingly, this relationship has found very few applications in the numerical analysis literature despite being well known. In this work, we leverage the important distinction between the Schrödinger and Hamilton-Jacobi equations, namely, that the former is linear whereas the latter is not. We take advantage of the linearity of the Schrödinger equation while exploiting its relationship to Hamilton-Jacobi and derive computationally efficient solutions to the eikonal equation.

Since the efficient solution of a linear wave equation is the cornerstone of our approach, we now briefly describe the actual computational algorithm used. We derive the static Schrödinger equation for the eikonal problem. The result is a generalized, screened Poisson equation [18] whose solution is known at $K$ seed points. This linear equation does not have a closed-form solution and therefore we resort to a perturbation method [17] of solution—which is related to the Born expansion [30]. The perturbation method comprises a sequence of multiplications with a space-varying forcing function followed by convolutions with a (modified) Green’s function (for the screened Poisson operator) which we solve using an efficient Fast Fourier transform (FFT)-based technique [7, 14]. Perturbation analysis involves a geometric series approximation for which we show convergence for all bounded forcing functions independent of the value of $\hbar$. 
1.2 Euclidean Distance Functions

In the special case where \( f(X) \) equals one everywhere, the solution to the eikonal equation is the Euclidean distance function \([33]\) and hence the Hamilton-Jacobi scalar field \( S \) satisfies the differential equation

\[
\| \nabla S(X) \| = 1. \tag{1-7}
\]

When we seek solution for \( S \) from a set of \( K \) discrete points \( \{Y_k\}_{k=1}^{K} \), the Euclidean distance problem can be formally stated as: Given a point-set \( Y = \{ Y_k \in \mathbb{R}^D, k \in \{1, ..., K\} \} \) where \( D \) is the dimensionality of the point-set and a set of equally spaced Cartesian grid points \( X \), the Euclidean distance function problem requires us to assign

\[
S(X) = \min_k \|X - Y_k\| \tag{1-8}
\]

where the norm \( \| . \| \) corresponds to the Euclidean distance.

All the aforementioned Hamilton-Jacobi solvers solves for \( S \) in Equation 1–7 by spatially discretizing the derivative operator based on the Godunov upwind discretization scheme \([50]\). A major advantage of our Schrödinger approach is that it does not require derivative discretization and this sometimes accounts for improved accuracy of our technique. Moreover Schrödinger formalism results in a closed-form solution for the Euclidean distance function problem and that it can be expressed as a discrete convolution and computed using a Fast Fourier Transform (FFT) \([7]\). However, a caveat is that our Euclidean distance function is an approximation since it is obtained for a small but non-zero value of Planck’s constant \( \hbar \), but nevertheless converges to the true solution as \( \hbar \to 0 \).

The Schrödinger equation approach gives us an unsigned distance function. We complement this by independently finding the sign of the distance function, by efficiently computing the winding number for each location in the 2D grid and its equivalent concept topological degree in 3D. We show that just as in the case of the Schrödinger
equation, the winding number and the topological degree computations can also be written in closed-form, expressed as a discrete convolution and computed using the FFT. This appears (to us at any rate) to be a novel contribution.

Furthermore, we often seek the gradient, divergence, curvature and medial axes of the signed distance function which are not easy to obtain by these Hamilton-Jacobi approaches due to the lack of differentiability of the signed distance function. But we can leverage the closed-form solution obtained from the Schrödinger to compute these quantities. Since our distance function is differentiable everywhere, we can once again write down closed-form expressions for the gradients and curvature, express them as discrete convolutions and again compute these quantities using FFTs. We visualize the gradients and the maximum curvature using 2D shape silhouettes as the source. The maximum curvature has a haunting similarity to the medial axes as shown in our experimental results. To our knowledge, the fast computation of the derivatives of the distance function on a regular grid using discrete convolutions is new.

1.3 Gradient Density Estimation

So far in our development on the relation between the wave function $\phi$ and the scalar field $S$, we expressed $S$ in the exponent of $\phi$. But when $S$ appears as the phase of the stationary wave function, instead of appearing in its exponent, specifically when

$$\phi(X) = \exp \left( \frac{iS(X)}{\hbar} \right),$$

as one finds in the WKB approximation of the eikonal equation [35], we noticed a surprising result relating the density of the gradients of $S (S_x, S_y)$ and the scaled power spectrum of the wave function for small values of $\hbar$. In other words the squared magnitude of the Fourier transform of the wave function is approximately equal to the density function of the gradients of $S$ with the approximation becoming increasingly exact as $\hbar \to 0$. Using stationary phase approximations—a well known technique in asymptotic analysis and standard integration techniques with proper ordering of limits,
we establish this gradient frequency relation for an arbitrary thrice differentiable function $S$ in one dimension and for distance transforms in two dimensions. We also furnish anecdotal visual evidences to corroborate our claim. The significance of our result is that "spatial frequencies become histogram bins”. Apart from providing with a new signature for the distance transforms, our result can be used to serve as its gradient density estimator. Since the density functions are obtained directly from the function $S$, our method circumvents the need to compute its derivative(s).
CHAPTER 2
CLASSICAL AND QUANTUM FORMULATION FOR THE EIKONAL EQUATION

2.1 Hamilton-Jacobi Formalism for the Eikonal Equation

2.1.1 Fermat’s Principle of Least Time

It is well known that the Hamilton-Jacobi equation formalism for the eikonal equation can be obtained by considering a variational problem based on Fermat’s principle of least time \[4\]. While we use \( D = 2 \) for illustration purposes, the approach is general and not restricted to a particular choice of dimension:

\[
I[q] = \int_{t_0}^{t_1} f(q_1, q_2) \sqrt{q_1'^2 + q_2'^2} \, dt. \tag{2–1}
\]

The variational problem defined above has its roots in geometric optics \[12\]. Consider a medium with refractive index \( f(q_1, q_2) \) and let a space curve \( \gamma \) be described by \((q_1(t), q_2(t), t), t \in [t_0, t_1]\). Fermat’s least time principle states that the necessary condition for \( \gamma \) to be a light ray is that \( I \) be an extremum. The quantity

\[
L(q_1, q_2, \dot{q}_1, \dot{q}_2, t) = f(q_1, q_2) \sqrt{\dot{q}_1^2 + \dot{q}_2^2} \tag{2–2}
\]

is called the optical Lagrangian. The generalized momenta are defined as \[22\]

\[
p_i \equiv \frac{\partial L}{\partial \dot{q}_i} = \frac{f \dot{q}_i}{\sqrt{\dot{q}_1^2 + \dot{q}_2^2}}. \tag{2–3}
\]

Since the Lagrangian is homogeneous of degree one in \((\dot{q}_1, \dot{q}_2)\), we cannot solve for \( \dot{q}_i \) as a function of \( p_i \). However the momentum variables \((p_i)\) satisfy the following relation, namely

\[
p_1^2 + p_2^2 = f^2 \tag{2–4}
\]

using which the eikonal equation is derived. A Legendre transformation \[3\] is used to obtain the Hamiltonian, which is given by

\[
H(q_1, q_2, p_1, p_2, t) = \sum_{i=1}^{2} p_i \dot{q}_i - L(q_1, q_2, \dot{q}_1, \dot{q}_2, t) \tag{2–5}
\]
where \( q_i \) is assumed to be a function of \( p_i \).

A Legendre transform is an operation that transforms one real-valued function into another in a way such that the derivative of the original function becomes the argument of the transformed function. It is easier to explain with functions of one variable. Consider a function \( g(x) \). Its Legendre transform \( g^* \) is defined as

\[
g^*(p) \equiv \max_x(px - g(x)). \tag{2–6}
\]

For a differentiable function \( g \), maximizing the above quantity over \( x \), gives us the relation

\[
g'(x) = p. \tag{2–7}
\]

Scenarios under which \( x \) can be expressed in terms of \( p \) using Equation 2–7, the Legendre function \( g^* \) can be obtained in closed form. Let \( x_0 \) be the location where the function \( px - g(x) \) attains its maximum. Then \( g^*(p) \) satisfies

\[
g(x_0) = g'(x_0)x_0 - g^*(p). \tag{2–8}
\]

From Equation 2–8, \( g^*(p) \) can be interpreted as the negative of the y-intercept of the tangent line to the graph of \( g \) that has slope \( p = g'(x_0) \). Without delving into further details, we basically transformed a function \( g \) defined on the variable \( x \), to a function \( g^* \) defined on \( p \) using Equation 2–7. The reader may refer to [3] to get a detailed explanation on Legendre transformations.

To obtain the Hamiltonian formulation from the Lagrangian formulation, we carried out something similar. The Lagrangian \( L \), defined in Equation 2–2, is a function of the positional coordinates \( q_i \) and its time derivative \( \dot{q}_i \). The Hamiltonian shifts the functional dependencies to the positions \( q_i \) and momenta \( p_i \) by defining \( p_i \) as in Equation 2–3 and expressing \( \dot{q}_i \) as a function of \( p'_i \)'s. Unfortunately in our case the Hamiltonian \( H \) cannot be expressed in closed form, as \( \dot{q}_i \) cannot be explicitly expressed as a function of \( p'_i \)'s.
The Hamilton-Jacobi equation is obtained via a canonical transformation \[22\] of the Hamiltonian. In classical mechanics, a canonical transformation is defined as a change of variables which leaves the form of the Hamiltonian unchanged. For a type 2 canonical transformation, we have

\[
\sum_{i=1}^{2} p_i q_i - H(q_1, q_2, p_1, p_2, t) = \sum_{i=1}^{2} P_i Q_i - K(Q_1, Q_2, P_1, P_2, t) + \frac{dF}{dt} \tag{2–9}
\]

where \( F \equiv - \sum_{i=1}^{2} Q_i P_i + F_2(q, P, t) \) which gives

\[
\frac{dF}{dt} = - \sum_{i=1}^{2} (Q_i P_i + Q_i \dot{P}_i) + \frac{\partial F_2}{\partial t} + \sum_{i=1}^{2} \left( \frac{\partial F_2}{\partial q_i} q_i + \frac{\partial F_2}{\partial P_i} P_i \right). \tag{2–10}
\]

When we pick a particular type 2 canonical transformation wherein \( \dot{P}_i = 0, i = 1, 2 \) and \( K(Q_1, Q_2, P_1, P_2, t) = 0 \), we get

\[
\frac{\partial F_2}{\partial t} + H(q_1, q_2, \frac{\partial F_2}{\partial q_1}, \frac{\partial F_2}{\partial q_2}, t) = 0 \tag{2–11}
\]

where we are forced to make the identification

\[
p_i = \frac{\partial F_2}{\partial q_i}, \quad i = 1, 2. \tag{2–12}
\]

Note that the new momenta \( P_i \) are constants of the motion (usually denoted by \( \alpha_i, i = 1, 2 \)). Changing \( F_2 \) to \( S^* \) as in common practice, we have the standard Hamilton-Jacobi equation for the function \( S^*(q_1, q_2, \alpha_1, \alpha_2, t) \), namely

\[
\frac{\partial S^*}{\partial t} + H(q_1, q_2, \frac{\partial S^*}{\partial q_1}, \frac{\partial S^*}{\partial q_2}, t) = 0. \tag{2–13}
\]
To complete the circle back to the Lagrangian, we take the total time derivative of the Hamilton-Jacobi function $S^*$ to get

\[
\frac{dS^*(q_1, q_2, \alpha_1, \alpha_2, t)}{dt} = \sum_{i=1}^{2} \frac{\partial S^*}{\partial q_i} \dot{q}_i + \frac{\partial S^*}{\partial t} = \sum_{i=1}^{2} p_i \dot{q}_i - H(q_1, q_2, \frac{\partial S^*}{\partial q_1}, \frac{\partial S^*}{\partial q_2}, t) = L(q_1, q_2, q_1, q_2, t). \tag{2–14}
\]

Consequently $S^*(q_1, q_2, \alpha_1, \alpha_2, t) = \int^t_{t_0} L dt$ and the constants $\{\alpha_1, \alpha_2\}$ can now be interpreted as integration constants. For a more accessible treatment of the relationship between Lagrangian's and the Hamilton-Jacobi field $S^*(q_1, q_2, \alpha_1, \alpha_2, t)$, please see [22]. Since the Hamiltonian is not an explicit function of time, Equation 2–13 can be simplified to the static Hamilton-Jacobi equation. By separation of variables, we get

\[
S^*(q_1, q_2, t) = S(q_1, q_2) - Et \tag{2–15}
\]

where $E$ is the total energy of the system and $S(q_1, q_2)$ is called Hamilton’s characteristic function [3]. Observing that $\frac{\partial S^*}{\partial q_i} = \frac{\partial S}{\partial q_i}$, and using the Equations 2–12 (replacing $F_2$ by $S$), and 2–4, we have $\| \nabla S \|^2 = f^2$, which is the familiar eikonal equation (Equation 1–1).

### 2.1.2 An Equivalent Variational Principle

We take an idiosyncratic approach to the eikonal equation by considering a different variational problem which is still very similar to Fermat’s least time principle. The advantage of this variational formulation is that the corresponding Schrödinger wave equation can be easily obtained.

Consider the following variational problem namely,

\[
I[q] = \int_{t_0}^{t_1} \frac{1}{2} (\dot{q}_1^2 + \dot{q}_2^2) f^2(q_1, q_2) dt \tag{2–16}
\]

where the Lagrangian $L$ is defined as

\[
L(q_1, q_2, q_1, q_2, t) \equiv \frac{1}{2} (\dot{q}_1^2 + \dot{q}_2^2) f^2(q_1, q_2). \tag{2–17}
\]
The above definition for \( L \) is actually the square of the Lagrangian considered in Equation 2–2. Squaring the Lagrangian makes it not to be homogeneous of degree one in \( \dot{q}_i \), allowing us to rewrite \( \dot{q}_i \) in terms of momentum variable \( p_i \), given by

\[
p_i \equiv \frac{\partial L}{\partial \dot{q}_i} = f^2(q_1, q_2) \dot{q}_i. \tag{2–18}
\]

It is worth emphasizing that minimizing \( l[q] \) in both the Equations 2–1 and 2–16 gives the same solution for \( q \). By applying the Legendre transformation [3] as before, we get a closed form expression for the Hamiltonian of the system in 2D as

\[
H(q_1, q_2, p_1, p_2, t) = \frac{1}{2} \left( \frac{p_1^2 + p_2^2}{f^2(q_1, q_2)} \right). \tag{2–19}
\]

From a canonical transformation of the Hamiltonian [22], we obtain the following Hamilton-Jacobi equation

\[
\frac{\partial S^*}{\partial t} + \frac{1}{2} \frac{\left( \frac{\partial S^*}{\partial q_1} \right)^2 + \left( \frac{\partial S^*}{\partial q_2} \right)^2}{f^2(q_1, q_2)} = 0 \tag{2–20}
\]

Since \( H \) is independent of time, by the separation of variables we can express

\[
S^*(q_1, q_2, t) = S(q_1, q_2) - Et. \]

Observing that \( \frac{\partial S^*}{\partial q_i} = \frac{\partial S}{\partial q_i} \), Equation 2–20 can be rewritten as

\[
\frac{1}{2} \left[ \left( \frac{\partial S}{\partial q_1} \right)^2 + \left( \frac{\partial S}{\partial q_2} \right)^2 \right] = Ef^2. \tag{2–21}
\]

Choosing the energy \( E \) to be \( \frac{1}{2} \), we obtain

\[
\| \nabla S \|^2 = f^2 \tag{2–22}
\]

which is the original eikonal equation (Equation 1–1). \( S \) is the required Hamilton-Jacobi scalar field which is efficiently obtained by the fast sweeping [50] and fast marching methods [34].
2.2 Schrödinger Wave Equation Formalism for the Eikonal Equation

In this section we derive a Schrödinger equation for our idiosyncratic variational problem (Equation 2–16) from first principles and then recover the scalar field $S$ [as in Equation 2–22] from the wave function.

2.2.1 A Path Integral Derivation of the Schrödinger Equation

Firstly, we consider the case where the forcing function $f$ is constant and equals $\tilde{f}$ everywhere and then generalize to spatially varying forcing functions. For constant forcing functions, the Lagrangian $L$ defined in Equation 2–17 is given by

$$L(q_1, q_2, \dot{q}_1, \dot{q}_2, t) = \frac{1}{2}(\dot{q}_1^2 + \dot{q}_2^2)\tilde{f}^2(q_1, q_2).$$  \hspace{1cm} (2–23)

We follow the Feynman path-integral approach [19, 44] to deriving the differential equation for the time-dependent wave function $\psi$ and subsequently arrive at the time-independent wave function $\phi$. We would like to emphasize that though the Feynman path integral approach gives a constructive mechanism for deriving the Schrödinger wave equation, it is not considered mathematically rigorous in the general setting. For a more detailed explanation on this subject, the reader may refer to [11, 19].

The key idea is to consider the transition amplitude (also called the short-time propagator) $K(X, t_2, \xi, t_1)$ where $KK^*$ corresponds to the conditional transitional probability density of a particle going from $\xi(t_1)$ to $X(t_2)$. For any specific path $X(t) = \{x_1(t), x_2(t)\}$ in 2D, the amplitude is assumed to be proportional to

$$\exp\left(\frac{i}{\hbar} \int_{t_1}^{t_2} L(X, \dot{X}, t) dt\right)$$  \hspace{1cm} (2–24)

where the Lagrangian $L$ is given by Equation 2–23. If the particle can move from $\xi$ to $X$ over a set of paths, the transition amplitude is defined as the sum of the amplitudes associated with each path, so

$$K(X, t_2; \xi, t_1) \equiv \int \exp\left(\frac{i}{\hbar} \int_{t_1}^{t_2} L(X, \dot{X}, t) dt\right) dX.$$  \hspace{1cm} (2–25)
Now suppose that a particle is moving from a starting position $X + \xi = (x_1 + \xi_1, x_2 + \xi_2)$ at time $t$ and ends at $x$ at time $t + \tau$ while traveling for a very short time interval $\tau$. Using the definition of the Lagrangian from Equation 2–17, the transition amplitude for this event is

$$K(X, t + \tau; X + \xi, t) = \int \exp \left( \frac{i}{\hbar} \int_{t}^{t+\tau} \left( \frac{1}{2} (x_1^2 + x_2^2) \tilde{\mathcal{E}}^2(x_1, x_2) dt' \right) \right) DX$$

$$\approx \int \exp \left\{ \int_{t}^{t+\tau} \left[ \left( \frac{\xi_1}{\tau} \right)^2 + \left( \frac{\xi_2}{\tau} \right)^2 \right] \tilde{\mathcal{E}}^2(x_1, x_2) \right\} DX$$

$$= M \exp \left\{ \frac{i}{2\hbar \tau} \left( \xi_1^2 + \xi_2^2 \right) \tilde{\mathcal{E}}^2(x_1, x_2) \right\}. \quad (2–26)$$

Here $M \equiv \int DX$. In order to derive the wave equation for $\psi$, we first recall that the wave function $\psi$ has an interpretation that $\psi^* \psi = |\psi(X, t)|^2$ denotes the probability of finding a particle at $X$ and at time $t$. Since $K$ behaves more like a conditional transitional probability from $X + \xi$ to $X$, the wave function should satisfy

$$\psi(X, t + \tau) = \int K(X, t + \tau; X + \xi, t) \psi(X + \xi, t) d\xi. \quad (2–27)$$

Expanding to the first order in $t$ and second order in $\xi$ we get

$$\psi + \tau \frac{\partial \psi}{\partial t} = \int M \exp \left\{ \frac{i}{2\hbar \tau} \left( \xi_1^2 + \xi_2^2 \right) \tilde{\mathcal{E}}^2(x_1, x_2) \right\}$$

$$\left[ \psi + \xi_1 \frac{\partial \psi}{\partial x_1} + \xi_2 \frac{\partial \psi}{\partial x_2} + \frac{\xi_1^2}{2} \frac{\partial^2 \psi}{\partial x_1^2} + \frac{\xi_2^2}{2} \frac{\partial^2 \psi}{\partial x_2^2} + \xi_1 \xi_2 \frac{\partial^2 \psi}{\partial x_1 \partial x_2} \right] d\xi$$

$$= l_1 \psi + l_2 \frac{\partial \psi}{\partial x_1} + l_3 \frac{\partial \psi}{\partial x_2} + l_4 \frac{1}{2} \frac{\partial^2 \psi}{\partial x_1^2} + l_5 \frac{1}{2} \frac{\partial^2 \psi}{\partial x_2^2} + l_6 \frac{\partial \psi}{\partial x_1} \frac{\partial \psi}{\partial x_2} \quad (2–28)$$
where the integrals $I_1, I_2, I_3, I_4, I_5, I_6$ are defined as

\[
    I_1 = M \int \int \exp \left\{ \frac{i}{2\hbar \tau} (\xi_1^2 + \xi_2^2) \tilde{F}^2(x_1, x_2) \right\} d\xi_1 d\xi_2,
\]

\[
    I_2 = M \int \int \exp \left\{ \frac{i}{2\hbar \tau} (\xi_1^2 + \xi_2^2) \tilde{F}^2(x_1, x_2) \right\} \xi_1 d\xi_1 d\xi_2,
\]

\[
    I_3 = M \int \int \exp \left\{ \frac{i}{2\hbar \tau} (\xi_1^2 + \xi_2^2) \tilde{F}^2(x_1, x_2) \right\} \xi_2 d\xi_1 d\xi_2,
\]

\[
    I_4 = M \int \int \exp \left\{ \frac{i}{2\hbar \tau} (\xi_1^2 + \xi_2^2) \tilde{F}^2(x_1, x_2) \right\} \xi_1^2 d\xi_1 d\xi_2,
\]

\[
    I_5 = M \int \int \exp \left\{ \frac{i}{2\hbar \tau} (\xi_1^2 + \xi_2^2) \tilde{F}^2(x_1, x_2) \right\} \xi_2^2 d\xi_1 d\xi_2,
\]

\[
    I_6 = M \int \int \exp \left\{ \frac{i}{2\hbar \tau} (\xi_1^2 + \xi_2^2) \tilde{F}^2(x_1, x_2) \right\} \xi_1 \xi_2 d\xi_1 d\xi_2.
\]  

(2–29)

Observing that the integral $I_2$ can be rewritten as a product of two integrals, i.e,

\[
    I_2 = M \int \exp \left\{ \frac{i}{2\hbar \tau} \xi_1^2 \tilde{F}^2(x_1, x_2) \right\} \xi_1 d\xi_1 \int \exp \left\{ \frac{i}{2\hbar \tau} \xi_2^2 \tilde{F}^2(x_1, x_2) \right\} d\xi_2
\]  

(2–30)

and that the first integral is an odd function of $\xi_1$, it follows that $I_2 = 0$. A similar argument shows that $I_3 = I_6 = 0$.

Using the relation

\[
    \int_{-\infty}^{\infty} \exp(i\alpha s^2) ds = \sqrt{\frac{i\pi}{\alpha}}
\]  

(2–31)

and noticing that $I_1$ can be written as a separate product of two integrals in $\xi_1$ and in $\xi_2$, it follows that

\[
    I_1 = M \frac{i2\hbar \tau \pi}{\tilde{F}^2(x_1, x_2)}.
\]  

(2–32)

In order for the equation for $\psi$ to hold, $I_1$ should approach 1 as $\tau \to 0$. Hence,

\[
    M = \frac{\tilde{F}^2(x_1, x_2)}{i2\hbar \tau \pi}.
\]  

(2–33)

Let $I$ denote the integral in Equation 2–31. Then

\[
    \frac{1}{i} \frac{\partial I}{\partial \alpha} = \frac{i}{2} \frac{\sqrt{i\pi}}{\alpha^{\frac{3}{2}}} = \int \exp(i\alpha s^2) s^2 ds.
\]  

(2–34)
Using the relations in Equations 2–31 and 2–34 with \( \alpha = \frac{\gamma^2}{2\kappa r} \) and writing \( l_4 \) and \( l_5 \) as product of two separate integrals in \( \xi_1 \) and \( \xi_2 \) and substituting the value of \( M \) from Equation 2–33, we obtain

\[
l_4 = l_5 = \frac{i\hbar\tau}{f^2(x_1, x_2)}. \tag{2–35}
\]

Substituting back the value of these integrals in Equation 2–28, we get

\[
\psi + i\frac{\partial\psi}{\partial t} = \psi + \frac{i\hbar}{2\hbar^2} \left( \frac{\partial^2 \psi}{\partial x_1^2} + \frac{\partial^2 \psi}{\partial x_2^2} \right) \tag{2–36}
\]

from which we obtain the Schrödinger wave equation [24]

\[
\frac{i\hbar}{\partial t} \frac{\partial \psi}{\partial t} = \hat{H}\psi \tag{2–37}
\]

where the Hamiltonian operator \( \hat{H} \) is given by

\[
\hat{H} = -\frac{\hbar^2}{2\hbar^2} \left( \frac{\partial^2 \psi}{\partial x_1^2} + \frac{\partial^2 \psi}{\partial x_2^2} \right). \tag{2–38}
\]

Since the Hamiltonian \( H \) doesn’t explicitly depend on time, using separation of variables \( \psi(X, t) = \phi(X)g(t) \), we get

\[
\frac{i\hbar}{\partial t} \frac{d\hat{g}}{g} = -\frac{\hbar^2}{2\hbar^2} \nabla^2 \phi = E \tag{2–39}
\]

where \( E \) is the energy state of the system and \( \nabla^2 \) is the Laplacian operator. Solving for \( g \), we get

\[
g(t) = \exp\left(\frac{Et}{i\hbar}\right) \tag{2–40}
\]

and \( \phi \) satisfies

\[
-\frac{\hbar^2}{2\hbar^2} \nabla^2 \phi = E\phi. \tag{2–41}
\]

The solution for the Schrödinger wave \( \psi \) is then of the form

\[
\psi(X, t) = \phi(X) \exp\left(\frac{Et}{i\hbar}\right). \tag{2–42}
\]
We are primarily interested in solving for $\phi$ and relate the stationary wave function $\phi$ and the Hamilton-Jacobi scalar field $S$ to obtain the solution for the latter.

When $E > 0$ in Equation 2–41, the solutions for $\phi$ are oscillatory in nature and when $E < 0$ the solutions are generalized functions (distributions) which are exponential in nature. This nature of the solution will become clearer when we provide the actual closed-form expression for the wave function in Section 3.1. For eikonal problems, we are primarily interested only in the exponential solution for $\phi$ computed at $E = -\frac{1}{2}$, as it allows us to explicitly show the convergence of our closed-form solution (obtained for constant forcing functions) to the true solution as $\hbar \to 0$. The reader may refer to Section 3.2 for detailed convergence proofs. Setting $E = -\frac{1}{2}$ in Equation 2–41, we get the Schrödinger wave equation where the wave function $\phi$ satisfies the differential equation

$$-\hbar^2 \nabla^2 \phi + \tilde{f}^2 \phi = 0. \quad (2–43)$$

Even for an arbitrary positive, bounded forcing function $f$, we propose to solve a differential equation very similar to Equation 2–43 by replacing the constant force $\tilde{f}$ with the spatially varying forcing function $f$. The Schrödinger wave equation for the general eikonal problem can then be stated as

$$-\hbar^2 \nabla^2 \phi + f^2 \phi = 0. \quad (2–44)$$

We would like to point out that the proposed wave equation (Equation 2–44) for the general eikonal equation can be derived from first principles based on the Feynman path integral approach by replacing $\tilde{f}$ by $f$ and exactly following the steps delineated above. The only caveat in the derivation being that the Hamiltonian operator defined in Equation 2–38 will no longer be self-adjoint and hence may not behave as the quantum mechanical operator corresponding to total energy of the physical system [24]. Nevertheless we show that the wave equation (Equation 2–44) in the limit as $\hbar \to 0$ gives rise to the eikonal equation.
2.2.2 Obtaining the Eikonal Equation from the Schrödinger Equation

When the action $S$ and the wave function $\phi$ are related through the exponent, specifically

$$\phi(X) = \exp \left\{ \frac{-S(X)}{\hbar} \right\},$$  \hspace{1cm} (2–45)

and $\phi$ satisfies Equation 2–44, we see that $S$ satisfies the eikonal equation (Equation 1–1) as $\hbar \rightarrow 0$. This relationship (Equation 2–45) can also be seen in the WKB approximation of the wave function to obtain the eikonal equation [35]. Since solutions to Equation 2–44 are real-valued functions [16], we had $S$ appearing in the exponent of $\phi$. For differential equations where solutions to $\phi$ are complex and oscillatory—corresponding to positive energy $E$ in Equation 2–41—$S$ appears as the phase of $\phi$, specifically $\phi(X) = \exp \left\{ \frac{i}{\hbar}S(X) \right\}$ as one finds in the WKB approximation. Chapter 6 is entirely devoted to this phase relationship between the wave function $\phi$ and the scalar field $S$ and its applications to estimation of gradient densities of $S$.

When $\phi(x_1, x_2) = \exp \left\{ \frac{-S(x_1, x_2)}{\hbar} \right\}$, the first partials of $\phi$ are

$$\frac{\partial \phi}{\partial x_1} = \frac{-1}{\hbar} \exp \left( \frac{-S}{\hbar} \right) \frac{\partial S}{\partial x_1}, \quad \frac{\partial \phi}{\partial x_2} = \frac{-1}{\hbar} \exp \left( \frac{-S}{\hbar} \right) \frac{\partial S}{\partial x_2}. \hspace{1cm} (2–46)$$

The second partials required for the Laplacian are

$$\frac{\partial^2 \phi}{\partial x_1^2} = \frac{1}{\hbar^2} \exp \left( \frac{-S}{\hbar} \right) \left( \frac{\partial S}{\partial x_1} \right)^2 - \frac{1}{\hbar} \exp \left( \frac{-S}{\hbar} \right) \frac{\partial^2 S}{\partial x_1^2},$$

$$\frac{\partial^2 \phi}{\partial x_2^2} = \frac{1}{\hbar^2} \exp \left( \frac{-S}{\hbar} \right) \left( \frac{\partial S}{\partial x_2} \right)^2 - \frac{i}{\hbar} \exp \left( \frac{-S}{\hbar} \right) \frac{\partial^2 S}{\partial x_2^2}. \hspace{1cm} (2–47)$$

From this, Equation 2–44 can be rewritten as

$$\left( \frac{\partial S}{\partial x_1} \right)^2 + \left( \frac{\partial S}{\partial x_2} \right)^2 - \hbar \left( \frac{\partial^2 S}{\partial x_1^2} + \frac{\partial^2 S}{\partial x_2^2} \right) = f^2 \hspace{1cm} (2–48)$$

which in simplified form is

$$\| \nabla S \|^2 - \hbar \nabla^2 S = f^2. \hspace{1cm} (2–49)$$
The additional $\hbar \nabla^2 S$ term (relative to Equation 1–1) is referred to as the viscosity term [16, 34] which emerges naturally from the Schrödinger equation derivation—an intriguing result. Again, since $| \nabla^2 S|$ is bounded, as $\hbar \to 0$, Equation 2–49 tends to

$$\| \nabla S \|^2 = \tilde{f}^2$$

(2–50)

which is the original eikonal equation (Equation 1–1). This relationship motivates us to solve the linear Schrödinger equation (Equation 2–44) instead of the non-linear eikonal equation and then compute the scalar field $S$ via

$$S(X) = -\hbar \log \phi(X).$$

(2–51)
CHAPTER 3
EUCLIDEAN DISTANCE FUNCTIONS

The Euclidean distance function problem—more popularly referred to as distance transforms, is a special case of the general eikonal equation where the forcing function \( f(X) \) is identically equal to one. Hence the Hamilton-Jacobi scalar field \( S \) satisfies the relation

\[
\| \nabla S \| = 1.
\] (3–1)

When we seek solution for \( S \) from a set of \( K \) discrete points \( \{ Y_k \}^{K}_{k=1} \) on a discretized spatial grid, the unsigned Euclidean distance problem can be formally stated as: Given a point-set \( Y = \{ Y_k \in \mathbb{R}^D, k \in \{1, ..., K\} \} \) where \( D \) is the dimensionality of the point-set and a set of equally spaced Cartesian grid points \( X \), the Euclidean distance function problem requires us to assign

\[
S(X) = \min_k \| X - Y_k \| \quad (3–2)
\]

with the Euclidean norm used in Equation 3–2. In computational geometry, this is the Voronoi problem [5] and the solution \( S(X) \) can be visualized as a set of cones (with the centers being the point-set locations \( \{ Y_k \} \)).

The analysis for the Euclidean distance problem can be extended to eikonal equation with constant forcing function where \( \tilde{f} = \tilde{f} = \text{const.} \), \( \tilde{f} = 1 \) specializes for the Euclidean distance transform. In the subsequent sections we arrive at the closed-form solutions for the Schrödinger equation corresponding to constant forcing functions (Equation 2–43), show proofs of convergence to the true solution in the limit as \( \hbar \to 0 \) and also provide an efficient FFT-based numerical technique to compute the solution.

3.1 Closed-Form Solutions for Constant Forcing Functions

We now derive the closed-form solution for \( \phi(X) \) (in 1D, 2D and 3D) satisfying Equation 2–43 and hence for \( S(X) \) by Equation 2–51.
Recall that we are interested in solving for the eikonal problem only on a discretized spatial grid consisting of \( N \) grid locations from a set of \( K \) discrete point sources \( \{ Y_k \}_{k=1}^{K} \) where the distance function is defined to be zero, namely \( S(Y_k) = 0, \forall Y_k, k \in \{1, ..., K\} \). Hence it circumvents the need to determine the solution for \( S \) and for the wave function \( \phi \) at these source locations. Furthermore since the Hamiltonian operator \( \hat{H} = -\hbar^2 \nabla^2 + 1 \) is positive definite, i.e, all the eigen value of \( \hat{H} \) if they exist are strictly positive, the eigen system

\[
-\hbar^2 \nabla^2 \phi = (-\tilde{r}^2)\phi
\]

(3–3)

aiming at finding a non-trivial eigen function \( \phi \) with an eigen value of \(-\tilde{r}^2\) is insatiable. Hence we look for solutions which are generalized functions (distributions) by considering the forced version of the equation, namely

\[
-\hbar^2 \nabla^2 \phi + \tilde{r}^2 \phi = \sum_{k=1}^{K} \delta(X - Y_k).
\]

(3–4)

where we force the differential equation to be satisfied at all the grid locations except at the point source locations \( \{ Y_k \}_{k=1}^{K} \) where \( S \) is a-priori known to be zero.

Since it is meaningful to assume that \( S(X) \) goes to infinity for points at infinity, we can use Dirichlet boundary conditions \( \phi(X) = 0 \) at the boundary of an unbounded domain. Now using a Green’s function approach [2], we can write expressions for the solution \( \phi \). The Green’s function \( G \) satisfies the relation

\[
(-\hbar^2 \nabla^2 + \tilde{r}^2) G(X) = -\delta(X).
\]

(3–5)

The form of \( G \) various with dimensions and and its expression [2] in 1D, 2D and 3D over an unbounded domain with vanishing boundary conditions at \( \infty \) is given by,

**1D:**

\[
G(X, Y) = \frac{1}{2\hbar} \exp \left( -\frac{\tilde{r}|X - Y|}{\hbar} \right).
\]

(3–6)
\[ \begin{align*} 
\text{2D:} \\
G(X, Y) &= \frac{1}{2\pi h^2} K_0 \left( \frac{\tilde{r} \|X - Y\|}{h} \right) \\
&\approx \frac{\exp \left( \frac{-\tilde{r} \|X - Y\|}{h} \right)}{2h \sqrt{2\pi h^2 \|X - Y\|}}, \quad \frac{\|X - Y\|}{h} \gg 0.25 
\end{align*} \]

where \( K_0 \) is the modified Bessel function of the second kind.

\[ \text{3D:} \\
G(X, Y) = \frac{1}{4\pi h^2} \exp \left( \frac{-\tilde{r} \|X - Y\|}{h} \right). \tag{3-8} \]

The solutions for \( \phi \) can then be obtained by convolution

\[ \phi(X) = \sum_{k=1}^{K} G(X) \ast \delta(X - Y_k) = \sum_{k=1}^{K} G(X - Y_k). \tag{3-9} \]

from which \( S \) can be recovered using the Equation 2–51.

### 3.2 Proofs of Convergence to the True Distance Function

We now show that as \( h \to 0 \), \( S \) converges to the true solution \( r = \tilde{r} \min_k \|X - Y_k\| \)

for all grid points \( X \) except the source locations \( Y_k \).

**1D:** From Equation 2–51, we get

\[ S(X) = -h \log \sum_{k=1}^{K} \exp \left( \frac{-r \|X - Y_k\|}{h} \right) + h \log (2h). \tag{3-10} \]

Observe that

\[ S(X) \leq -h \log \exp \left( \frac{-r}{h} \right) + h \log(2h) \]

\[ = r + h \log(2h). \tag{3-11} \]

Also,

\[ S(X) \geq -h \log \left[ K \exp \left( \frac{-r}{h} \right) \right] + h \log(2h) \]

\[ = -h \log K + r + h \log(2h). \tag{3-12} \]
As \( h \to 0 \), \( h \log K \to 0 \) and \( h \log \dot{h} \to 0 \). Furthermore, we see from Equations 3–11 and 3–12 that

\[
\lim_{h \to 0} S(X) = r. \quad (3-13)
\]

2D: From Equation 2–51, we get

\[
S(X) = -h \log \sum_{k=1}^{K} K_0 \left( \frac{\tilde{f} ||X - Y_k||}{h} \right) + h \log(2\pi h^2). \quad (3-14)
\]

Then,

\[
S(X) \leq -h \log K_0 \left( \frac{f}{h} \right) + h \log(2\pi h^2). \quad (3-15)
\]

Using the relation \( K_0 \left( \frac{f}{h} \right) \geq \frac{\exp \left( -\frac{f}{h} \right)}{\sqrt{\pi}} \) when \( \frac{f}{h} \geq 0.5 \), we get

\[
S(X) \leq -h \log \left[ \frac{\sqrt{h}}{r} \exp \left( -\frac{r}{h} \right) \right] + h \log(2\pi h^2) = -h \log \sqrt{\frac{h}{r}} + r + h \log(2\pi h^2). \quad (3-16)
\]

Moreover

\[
S(X) \geq -h \log \left[ KK_0 \left( \frac{r}{h} \right) \right] + h \log(2\pi h^2). \quad (3-17)
\]

Using the relation \( K_0 \left( \frac{f}{h} \right) \leq \exp \left( -\frac{f}{h} \right) \) when \( \frac{f}{h} \geq 1.5 \), we get

\[
S(X) \geq -h \log \left[ K \exp \left( -\frac{r}{h} \right) \right] + h \log(2\pi h^2) = -h \log K + r + h \log(2\pi h^2). \quad (3-18)
\]

As \( h \to 0 \), \( h \log K \to 0 \), \( h \log r \to 0 \) and \( h \log \dot{h} \to 0 \). Furthermore, we see from Equations 3–16 and 3–18 that

\[
\lim_{h \to 0} S(X) = r. \quad (3-19)
\]

3D: From Equation 2–51,

\[
S(X) = -h \log \sum_{k=1}^{K} \frac{\exp \left( -\frac{\tilde{f} ||X - Y_k||}{h} \right)}{\tilde{f} ||X - Y_k||} + h \log \left( 4\pi h^2 \right). \quad (3-20)
\]
Then,

\[
S(X) \leq -\frac{h \log \left( \frac{-r}{h} \right)}{r} + h \log(4\pi h^2) \\
= r + h \log r + h \log \left( 4\pi h^2 \right).
\]  

(3–21)

Also,

\[
S(X) \geq -h \log \left[ K \frac{\exp \left( \frac{-\tilde{r}}{h} \right)}{r} \right] + h \log(4\pi h^2) \\
= -h \log K + r + h \log r + h \log(4\pi h^2).
\]  

(3–22)

As \( h \to 0 \), \( h \log K \to 0 \), \( h \log r \to 0 \) and \( h \log h \to 0 \). Furthermore, we see from Equations 3–21 and 3–22 that

\[
\lim_{h \to 0} S(X) = r.
\]  

(3–23)

Hence, we see that (in 1D, 2D and 3D), the closed form solution for \( \phi \) guarantees that \( S \) approaches the true function in the limit \( h \to 0 \).

### 3.3 Modified Green’s Function

Based on the nature of the Green’s function we would like to highlight on the following very important point. In the limiting case of \( h \to 0 \),

\[
\lim_{h \to 0} \exp \left\{ \frac{-\tilde{r} \|X\|}{h} \right\} \times \frac{1}{ch^d \|X\|^p} = 0, \text{ for } \|X\| \neq 0
\]  

(3–24)

for \( c, d \) and \( p \) being constants greater than zero and therefore we see that if we define

\[
\tilde{G}(X) = C \exp \left( \frac{-\tilde{r} \|X\|}{h} \right)
\]  

(3–25)

for some constant \( C \),

\[
\lim_{h \to 0} \|G(X) - \tilde{G}(X)\| = 0, \text{ for } \|X\| \neq 0
\]  

(3–26)

and furthermore, the convergence is uniform for \( \|X\| \) away from zero. Therefore, \( \tilde{G}(X) \) provides a very good approximation for the actual Green’s function as \( h \to 0 \). For a fixed value of \( h \) and \( X \), the difference between the Green’s functions is \( O \left( \frac{\exp \left( \frac{-\tilde{r} \|X\|}{h} \right)}{h^2} \right) \).
which is relatively insignificant for small values of $\hbar$ and for all $X \neq 0$. Moreover, using $\tilde{G}$ also avoids the singularity at the origin that $G$ has in the 2D and 3D case. The above observation motivates us to compute the solutions for $\phi$ by convolving with $\tilde{G}$, namely

$$
\phi(X) = \sum_{k=1}^{K} \tilde{G}(X) * \delta(X - Y_k) = \sum_{k=1}^{K} \tilde{G}(X - Y_k) \quad (3-27)
$$

instead of the actual Green’s function $G$ and recover $S$ using the Equation 2–51, given by

$$
S(X) = -\hbar \log \left[ \sum_{k=1}^{K} \exp \left( \frac{-\tilde{r} ||X - Y_k||}{\hbar} \right) \right] + \hbar \log(C). \quad (3-28)
$$

Since $\hbar \log(C)$ is a additive constant independent of $X$ and converges to 0 as $\hbar \to 0$, it can ignored while computing $S$ at small values of $\hbar$–it is equivalent to setting $C$ to be 1. Hence the Schrödinger wave function for constant forcing functions can be approximated by

$$
\phi(X) = \sum_{k=1}^{K} \exp \left( \frac{-\tilde{r} ||X - Y_k||}{\hbar} \right). \quad (3-29)
$$

It is worth emphasizing that the above defined wave function $\phi(X)$ (Equation 3–29), contains all the desirable properties that we need. Firstly, we notice that as $\hbar \to 0$, $\phi(Y_k) \to 1$ at the given point-set locations $Y_k$. Hence from Equation 2–51, $S(Y_k) \to 0$ as $\hbar \to 0$ satisfying the necessary initial conditions. Secondly as $\hbar \to 0$, $\sum_{k=1}^{K} \exp \left( \frac{-\tilde{r} ||X - Y_k||}{\hbar} \right)$ can be approximated by $\exp \left( \frac{-\tilde{r}}{\hbar} \right)$ where $r = \tilde{r} \min_k ||X - Y_k||$. Hence $S(X) \approx -\hbar \log \exp \left( \frac{-\tilde{r}}{\hbar} \right) = r$, which is the true value. Thirdly, $\phi$ can be easily computed using the fast Fourier transform as described under Section 3.5). Hence for all computational purposes we consider the wave function defined in Equation 3–29 as the solution to the Schrödinger wave equation (Equation 2–43).
3.4 Error Bound Between the Obtained and the True Distance Function

Using the Equation 2–51 and the modified Green’s function ($\tilde{G}$) we compute the approximate distance function as

$$S(X) = -\bar{h} \log \left( \sum_{k=1}^{K} \exp \left( -\frac{\tilde{f} \|X - Y_k\|}{\bar{h}} \right) \right). \quad (3–30)$$

Intuitively, as $\bar{h} \to 0$, $\sum_{k=1}^{K} \exp \left( -\frac{\tilde{f} \|X - Y_k\|}{\bar{h}} \right)$ can be approximated by $\exp \left( \frac{-r}{\bar{h}} \right)$ where $r = \tilde{f} \min_k \|X - Y_k\|$. Hence $S(X) \approx -\bar{h} \log \exp \left( \frac{-r}{\bar{h}} \right) = r$. The bound derived below between $S(X)$ and $r$ also unveils the proximity between the computed and the actual distance function. Note from Equation 3–30 that

$$S(X) \leq -\bar{h} \log \exp \left( \frac{-r}{\bar{h}} \right) = r. \quad (3–31)$$

Also, observe that

$$S(X) \geq -\bar{h} \log \left[ K \exp \left( \frac{-r}{\bar{h}} \right) \right]$$
$$= -\bar{h} \log K + r \quad (3–32)$$

and hence,

$$r - S(X) \leq \bar{h} \log K. \quad (3–33)$$

From Equations 3–31 and 3–33,

$$|r - S(X)| \leq \bar{h} \log K. \quad (3–34)$$

Equation 3–34 shows that as $\bar{h} \to 0$, $S(X) \to r$. It is worth commenting that the bound $\bar{h} \log K$ is actually very tight as (i) it scales only as the logarithm of the cardinality of the point-set ($K$) and (ii) it can be made arbitrarily small by choosing a small but non-zero value of $\bar{h}$. 
Table 3-1. Algorithm for the approximate Euclidean distance function

1. Compute the function $\tilde{G}(X) = \exp \left( -\frac{\|X\|}{h} \right)$ at the grid locations.
2. Define the function $\delta_{\text{kron}}(X)$ which takes the value 1 at the point-set locations and 0 at other grid locations.
3. Compute the FFT of $\tilde{G}$ and $\delta_{\text{kron}}$, namely $\tilde{G}_{\text{FFT}}(U)$ and $\delta_{\text{FFT}}(U)$ respectively.
4. Compute the function $H(U) = \tilde{G}_{\text{FFT}}(U)\delta_{\text{FFT}}(U)$.
5. Compute the inverse FFT of $H$ to obtain $\phi(X)$ at the grid locations.
6. Take the logarithm of $\phi(X)$ and multiply it by $(-h)$ to get the approximate Euclidean distance function at the grid locations.

3.5 Efficient Computation of the Approximate Distance Function

In this section, we provide numerical techniques for efficiently computing the wave function. Recall that we are interested in solving the eikonal equation only at the given $N$ discrete grid locations. In order to obtain the desired solution for $\phi$ (Equation 3–29) computationally, we must replace the $\delta$ function by the Kronecker delta function

$$\delta_{\text{kron}}(X) = \begin{cases} 
1 & \text{if } X = Y_k; \\
0 & \text{otherwise}
\end{cases}$$

that takes 1 at the point-set locations ($\{Y_k\}$) and 0 at other grid locations. Then $\phi$ can be exactly computed at the grid locations by the discrete convolution of $\tilde{G}$ (setting $C = 1$) with the Kronecker-delta function. By the convolution theorem [7], a discrete convolution can be obtained as the inverse Fourier transform of the product of two individual transforms which for two $O(N)$ sequences can be performed in $O(N \log N)$ time [14].

One just needs to compute the discrete Fourier transform (DFT) of $\tilde{G}$ and $\delta_{\text{kron}}$, compute their point-wise product and then compute the inverse discrete Fourier transform. Taking the logarithm of the inverse discrete Fourier transform and multiplying it by $(-h)$, gives the approximate Euclidean distance function. The algorithm is adumbrated in Table 3-1.

3.5.1 Solution for the Distance Function in Higher Dimensions

Using $\tilde{G}$ instead of the bounded domain Green’s function $G$ provides a straightforward generalization of our technique to higher dimensions. Regardless of the spatial dimension, the approximate solution for the distance function $S$ can be computed
from the wave function $\phi$ using $O(N \log N)$ floating-point operations as implementing
the discrete convolution using FFT [7] always involves $O(N \log N)$ floating-point
computations [14] irrespective of the spatial dimension. Though the number of grid
points($N$) may increase with dimension the solution is always $O(N \log N)$ in the number
of grid points. This speaks for the scalability of our technique.

3.5.2 Numerical Issues and Exact Computational Complexity

We request the reader to refer to Section 5.3.1 to get an account on the numerical
issues involved in computing the wave function and the need for arbitrary precision
arithmetic packages like GMP and MPFR [20, 45]. Moreover the $O(N \log N)$ time
complexity of the FFT algorithm [14] for an $O(N)$ length sequence takes into account
only the number of floating-point operations involved, barring any numerical accuracy.
Section 5.3.2 gives the exact computational complexity, when one takes into account the
number of precision bits used in floating point computations.
The solution for the approximate Euclidean distance function in (3–30) (with \(\tilde{r} = 1\)) is lacking in one respect: there is no information on the sign of the distance. This is to be expected since the distance function was obtained only from a set of points \(\{Y_k\}_{k=1}^k\) and not a curve or a surface. We now describe a new method for computing the signed distance in 2D using winding numbers and in 3D using topological degree. Furthermore just as the approximate Euclidean distance function \(S(X)\) can be efficiently computed, so can the derivatives. This is important because fast computation of the derivatives of \(S(X)\) on a regular grid can be very useful in medial axis and curvature computations.

4.1 Convolution Based Method for Computing the Winding Number

Assume that we have a closed, parametric curve \(\{x^{(1)}(t), x^{(2)}(t)\}, t \in [0, 1]\). We seek to determine if a grid location in the set \(\{X_i \in \mathbb{R}^2, i \in \{1, \ldots, N\}\} \) is inside the closed curve. The winding number is the number of times the curve winds around the point \(X_i\) (if at all) and if the curve is oriented, counterclockwise turns are counted as positive and clockwise turns as negative. If a point is inside the curve, the winding number is a non-zero integer. If the point is outside the curve, the winding number is zero. If we can efficiently compute the winding number for all points on a grid w.r.t. to a curve, then we would have the sign information (inside/outside) for all the points. We now describe a fast algorithm to achieve this goal.

If the curve is \(C^1\), then the angle \(\theta(t)\) of the curve is continuous and differentiable and \(d\theta(t) = \left(\frac{x^{(1)}x^{(2)} - x^{(2)}x^{(1)}}{\|x\|^2}\right)dt\). Since we need to determine whether the curve winds around each of the points \(X_i, i \in \{1, \ldots, N\}\), define \((\hat{x}_i^{(1)}, \hat{x}_i^{(2)}) \equiv (x^{(1)} - X_i^{(1)}, x^{(2)} - X_i^{(2)}), \forall i\). Then the winding numbers for all grid points in the set \(X\) are

\[
\mu_i = \frac{1}{2\pi} \oint_C \left(\frac{\hat{x}_i^{(1)}\hat{x}_i^{(2)} - \hat{x}_i^{(2)}\hat{x}_i^{(2)}}{\|\hat{x}_i\|^2}\right) dt, \forall i \in \{1, \ldots, N\}.
\] (4–1)
As it stands, we cannot actually compute the winding numbers without performing the integral in Equation 4–1. To this end, we discretized the curve and produce a sequence of points \( \{ Y_k \in \mathbb{R}^2, k \in \{1, \ldots, K\} \} \) with the understanding that the curve is closed and therefore the “next” point after \( Y_K \) is \( Y_1 \). (The winding number property holds for piecewise continuous curves as well.) The integral in Equation 4–1 becomes a discrete summation and we get

\[
\mu_i = \frac{1}{2\pi} \sum_{k=1}^{K} \frac{\left( Y_k^{(1)} - X_i^{(1)} \right) \left( Y_k^{(2)} - Y_k^{(2)} \right) - \left( Y_k^{(2)} - X_i^{(2)} \right) \left( Y_k^{(1)} - Y_k^{(1)} \right)}{\| Y_k - X_i \|^2} \tag{4–2}
\]

\( \forall i \in \{1, \ldots, N\} \), where the notation \( Y_k^{(i)} \) denotes that \( Y_k^{(i)} = Y_{k+1}^{(i)} \) for \( k \in \{1, \ldots, K-1\} \) and \( Y_K^{(i)} = Y_1^{(i)} \). We can simplify the notation in Equation 4–2 (and obtain a measure of conceptual clarity as well) by defining the “tangent” vector \( \{ Z_k, k = \{1, \ldots, K\} \} \) as

\[
Z_k^{(i)} = Y_k^{(i)} - Y_k^{(i)}, \quad k \in \{1, \ldots, K\} \tag{4–3}
\]

with the \( (\cdot) \) symbol indicating either coordinate. Using the tangent vector \( Z \), we rewrite Equation 4–2 as

\[
\mu_i = \frac{1}{2\pi} \sum_{k=1}^{K} \frac{\left( Y_k^{(1)} - X_i^{(1)} \right) Z_k^{(2)} - \left( Y_k^{(2)} - X_i^{(2)} \right) Z_k^{(1)}}{\| Y_k - X_i \|^2}, \quad \forall i \in \{1, \ldots, N\} \tag{4–4}
\]

We now make the somewhat surprising observation that \( \mu \) in Equation 4–4 is a sum of two discrete convolutions. The first convolution is between two functions \( f_{cr}(X) \equiv f_c(X)f_r(X) \) and \( g_2(X) = \sum_{k=1}^{K} Z_k^{(2)} \delta_{\text{kron}} \) where the Kronecker delta function \( (\delta_{\text{kron}}) \) is defined in Equation 3.5. The second convolution is between two functions \( f_{sr}(X) \equiv f_s(X)f_r(X) \) and \( g_1(X) = \sum_{k=1}^{K} Z_k^{(1)} \delta_{\text{kron}} \). The functions \( f_c(X), f_s(X) \) and \( f_r(X) \) are defined as

\[
f_c(X) \equiv \frac{X^{(1)}}{\|X\|}, \quad f_s(X) \equiv \frac{X^{(2)}}{\|X\|}, \quad \text{and} \tag{4–5}
\]

\[
\frac{1}{\|X\|} \tag{4–6}
\]
with the understanding that \( f_c(0) = f_s(0) = f_r(0) = 0 \). Here we have abused notation somewhat and let \( X^{(1)} (X^{(2)}) \) denote the \( x \) (\( y \))-coordinate of all the points in the grid set \( X \). Armed with these relationships, we rewrite Equation 4–4 to get

\[
\mu(X) = \frac{1}{2\pi} \left[ -f_{cr}(X) * g_2(X) + f_{sr}(X) * g_1(X) \right]
\] (4–7)

which can be simultaneously computed for all the \( N \) grid points \( X_i \) using two FFTs.

### 4.2 Convolution Based Method for Computing the Topological Degree

The winding number concept for 2D admits a straightforward generalization to 3D and higher dimensions. The equivalent concept is the topological degree which is based on normalized flux computations. Assume that we have an oriented surface in 3D [23] which is represented as a set of \( K \) triangles. Each \( k^{th} \) triangle has an outward pointing normal \( P_k \) and this can easily be obtained once the surface is oriented. (We vectorize the edge of each triangle. Since triangles share edges, if the surface can be oriented, then there’s a consistent way of lending direction to each triangle edge. The triangle normal is merely the cross product of the triangle vector edges.) We pick a convenient triangle center (the triangle incenter for instance) for each triangle and call it \( Y_k \). The normalized flux (which is very closely related to the topological degree) [1] determines the ratio of the outward flux from a point \( X_i \) treated as the origin. If \( X_i \) is outside the enclosed surface, then the total outward flux is zero. If the point is inside, the outward normalized flux will be non-zero and positive.

The normalized flux for a point \( X_i \) is

\[
\mu_i = \frac{1}{4\pi} \sum_{k=1}^{K} \frac{\langle (Y_k - X_i), P_k \rangle}{\|Y_k - X_i\|^3}.
\] (4–8)

This can be written in the form of convolutions. To see this, we write Equation 4–8 in component form,

\[
\mu_i = \frac{1}{4\pi} \sum_{k=1}^{K} \frac{(Y_k^{(1)} - X_i^{(1)})P_k^{(1)} + (Y_k^{(2)} - X_i^{(2)})P_k^{(2)} + (Y_k^{(3)} - X_i^{(3)})P_k^{(3)}}{\|Y_k - X_i\|^3}
\] (4–9)
which can be simplified as

\[ \mu(X) = -\frac{1}{4\pi} (f_1(X) * g_1(X) + f_2(X) * g_2(X) + f_3(X) * g_3(X)) \]  

where \( f_i(X) \equiv \frac{x_i}{\|X\|} \) and \( g_i(X) \equiv \sum_{k=1}^{K} P_k^{(i)} \delta_{kron} \), where the Kronecker delta function \( (\delta_{kron}(X)) \) is given by Equation 3.5. This can be simultaneously computed using three FFTs for all the \( N \) grid points \( X \).

For the sake of clarity, we explicitly show the generalization of the winding number to the topological degree by rewriting some of the calculations involved in computing the winding number. Recall that for every point \( Y_k \) on the discretized curve, we defined its tangent vector \( Z_k \) as in Equation 4–3. The outward pointing normal \( P_k = (P_k^{(1)}, P_k^{(2)}) \), at the point \( Y_k \) (\( P_k \) will point outwards provided \( Y_1, Y_2, \cdots, Y_k \) are taken in the anti-clockwise order), is given by \( P_k^{(1)} = Z_k^{(2)}, P_k^{(2)} = -Z_k^{(1)} \). Using the normal vector \( P_k \), Equation 4–4 can be rewritten as

\[ \mu_i = \frac{1}{2\pi} \sum_{k=1}^{K} \frac{\langle (Y_k - X_i), P_k \rangle}{\|Y_k - X_i\|^2}. \]  

(4–11)

Notice the similarity between the Equations 4–11 and 4–8. The generalization is quite obvious.

Thus we have shown that the sign component of the Euclidean distance function can be separately computed (without knowledge of the distance) in parallel in using FFT’s on a regular 2D and 3D grid.

### 4.3 Fast Computation of the Derivatives of the Distance Function

As mentioned before, even the derivatives of Euclidean distance function \( S(X) \) can be represented as convolutions and efficiently computed using FFT’s. Below, we detail how this can be achieved. We begin with the gradients and for illustration purposes, the
derivations are performed in 2D:

\[ S_x(X) = \frac{1}{\sum_{k=1}^{K} \exp \left\{ -\frac{\|X-Y_k\|}{h} \right\}} \sum_{k=1}^{K} \frac{f_c(X-Y_k) \exp \left\{ -\frac{\|X-Y_k\|}{h} \right\}}{f(X) * \delta_{\text{kron}}(X)}. \]  (4–12)

A similar expression can be obtained for \( S_y(X) \). These first derivatives can be rewritten as discrete convolutions:

\[ S_x(X) = \frac{f_c(X) * \delta_{\text{kron}}(X)}{f(X) * \delta_{\text{kron}}(X)}, \quad S_y(X) = \frac{f_s(X) * \delta_{\text{kron}}(X)}{f(X) * \delta_{\text{kron}}(X)}. \]  (4–13)

where \( f_c(X) \) and \( f_s(X) \) are as defined in Equation 4–5, the Kronecker delta function \( (\delta_{\text{kron}}(X)) \) is given by Equation 3.5 and

\[ f(X) = \exp \left( \frac{-\bar{r} \|X\|}{h} \right) \]  (4–14)

is the modified Green’s function \( \bar{G} \) (defined in Equation 3–25) with the constant \( C = 1 \).

The second derivative formulae are somewhat involved. Rather than hammer out the algebra in a turgid manner, we merely present the final expressions—all discrete convolutions—for the three second derivatives in 2D:

\[ S_{xx}(X) = \frac{\left[ -\frac{1}{h} f_c^2(X) + f_s^2(X)f_r(X) \right] f(X) * g(X)}{f(X) * g(X)} + \frac{1}{h} (S_x)^2(X), \]  \hspace{1cm} (4–15)

\[ S_{yy}(X) = \frac{\left[ -\frac{1}{h} f_s^2(X) + f_c^2(X)f_r(X) \right] f(X) * g(X)}{f(X) * g(X)} + \frac{1}{h} (S_y)^2(X), \]  \hspace{1cm} (4–16)

\[ S_{xy}(X) = -\frac{\left[ \frac{1}{h} + f_r(X) \right] f_c(X)f_s(X)f(X) * g(X)}{f(X) * g(X)} + \frac{1}{h} S_x(X)S_y(X) \]  \hspace{1cm} (4–17)

where \( f_r(X) \) is as defined in Equation 4–6. We also see that

\[ \| \nabla S \|^2 - h^2 S = 1 - h f_r(X)f(X) * g(X) \]  \hspace{1cm} (4–19)
[since $t_c^2(X) + t_s^2(X) = 1$] with the right side going to one as $\alpha \to 0$ for points $X$ away from points in the seed point-set $\{Y_k\}_{k=1}^K$. This is in accordance with Equation 2–49 and vindicates our choice of the replacement Green’s function in Equation 3–25.

Since we can efficiently compute the first and second derivatives of the approximate Euclidean distance function everywhere on a regular grid, we can also compute derived quantities such as curvature (Gaussian, mean and principal curvatures) for the two-dimensional surface $S(X)$ computed at the grid locations $X$. In the experimental section, we visualize the derivatives and maximum curvature for shape silhouettes and use them as a vehicle to determine the medial axis for these silhouettes.
CHAPTER 5
GENERAL EIKONAL EQUATION

In this chapter, we provide numerical techniques for efficiently solving the Schrödinger equation (Equation 2–44) derived for an arbitrary, spatially varying, positive valued, bounded forcing function \( f \).

5.1 Perturbation Theory

When \( f \) is constant as in the case of Euclidean distance function problem (where it is identically equal to one), we showed the existence of closed-form solutions for the wave function \( \phi \) in Chapter 3. But for arbitrary forcing functions \( f \) which is what we face in the case of the eikonal, it is generally not true. Consequently, we propose to solve the linear system Equation 2–44 using techniques from perturbation theory [17].

Assuming that \( f \) is close to a constant non-zero forcing function \( \tilde{f} \), Equation 2–44 can be rewritten as

\[
(-\hbar^2 \nabla^2 + \tilde{f}^2) \left[ 1 + (-\hbar^2 \nabla^2 + \tilde{f}^2)^{-1} \circ (f^2 - \tilde{f}^2) \right] \phi = 0.
\]

Now, defining the operator \( L \) as

\[
L \equiv (-\hbar^2 \nabla^2 + \tilde{f}^2)^{-1} \circ (f^2 - \tilde{f}^2)
\]

and \( \phi_0 \) as

\[
\phi_0 \equiv (1 + L)\phi
\]

we see that \( \phi_0 \) satisfies

\[
(-\hbar^2 \nabla^2 + \tilde{f}^2)\phi_0 = 0
\]

and

\[
\phi = (1 + L)^{-1}\phi_0.
\]

Notice that in the differential equation for \( \phi_0 \) (Equation 5–4), the forcing function is constant and equals \( \tilde{f} \) everywhere. Hence \( \phi_0 \) behaves like the wave function

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corresponding to the constant forcing function \( \tilde{f} \) and can be approximated by

\[
\phi_0(X) = \sum_{k=1}^{K} \exp \left( -\tilde{f} \frac{\|X - Y_k\|}{h} \right)
\] (5–6)

(refer Equation 3–29).

We now solve for \( \phi \) in Equation 5–5 using a geometric series approximation for \((1 + L)^{-1}\). Firstly, observe that the approximate solution for \( \phi_0 \) in Equation 5–6 is a square-integrable function which is necessary for the subsequent steps.

Let \( \mathcal{H} \) denote the space of square integrable functions on \( \mathbb{R}^D \), i.e, \( g \in \mathcal{H} \) iff

\[
\int g^2 d\mu < \infty.
\] (5–7)

The function norm \( \|g\| \) for a function \( g \in \mathcal{H} \) is given by

\[
\|g\|^2 = \int g^2 d\mu.
\] (5–8)

Let \( B \) denote a closed unit ball in the Hilbert space \( \mathcal{H} \), i.e

\[
B = \{ g \in \mathcal{H} : \|g\| \leq 1 \}.
\] (5–9)

Let \( c_0 \equiv \|L\|_{\text{op}} \)—the operator norm—defined by

\[
c_0 = \sup \{ \|Lg\|, \forall \text{functions } g \in B \}.
\] (5–10)

If \( c_0 < 1 \), we can approximate \((1 + L)^{-1}\) using the first few \( T + 1 \) terms of the geometric series to get

\[
(1 + L)^{-1} \approx 1 - L + L^2 - L^3 + \ldots + (-1)^T L^T
\] (5–11)

where the operator norm of the difference can be bounded by

\[
\|(1 + L)^{-1} - \sum_{i=0}^{T} (-1)^i L^i\|_{\text{op}} \leq \sum_{i=T+1}^{\infty} \|L^i\|_{\text{op}} \leq \sum_{i=T+1}^{\infty} c_0^i = \frac{c_0^{T+1}}{1 - c_0}
\] (5–12)
which converges to 0 exponentially in $T$. We would like to point out that the above geometric series approximation is similar to a Born expansion used in scattering theory [30]. We now derive an upper bound for $c_0$.

Let $L = A_1 \circ A_2$ where $A_1 \equiv (-h^2 \nabla^2 + \vec{r}^2)^{-1}$ and $A_2 \equiv \vec{f}^2 - \vec{r}^2$. We now provide an upper bound for $\|A_1\|_{op}$.

For a given $g \in B$, let $z = A_1(g)$, i.e $z$ satisfies the relation

\[
(-h^2 \nabla^2 + \vec{r}^2)z = g
\]

with vanishing Dirichlet boundary conditions at $\infty$. Then

\[
\|(-h^2 \nabla^2 + \vec{r}^2)z\|^2 = \| - h^2 \nabla^2 z\|^2 + \|\vec{r}^2 z\|^2 + 2h^2 \vec{r}^2 (z \nabla^2 z, z) = \|g\|^2 \leq 1. \tag{5–14}
\]

We now use the relation

\[
\nabla \cdot (z \nabla z) = z \nabla^2 z + |\nabla z|^2
\]

(5–15)

to compute

\[
\langle - \nabla^2 z, z \rangle = - \int z \nabla^2 zd\mu = - \int \nabla \cdot (z \nabla z) d\mu + \int |\nabla z|^2 d\mu. \tag{5–16}
\]

Now from the divergence theorem we have

\[
- \int \nabla \cdot (z \nabla z) d\mu = 0 \quad \tag{5–17}
\]

and hence

\[
\langle - \nabla^2 z, z \rangle = \int |\nabla z|^2 d\mu \geq 0. \tag{5–18}
\]

Using the above relation in Equation 5–14, we then observe that

\[
\|z\| = \|A_1(g)\| \leq \frac{1}{f^2}, \forall g \in B. \tag{5–19}
\]
Since we showed $A_1(B)$ is bounded and less than or equal to $\frac{1}{f^2}$, we immediately have
\[ \|A_1\|_{op} \leq \frac{1}{f^2}. \] (5–20)

Now, let $M = \sup\{|f^2 - \tilde{f}^2|\}$. Then, for any $g \in B$
\[ \|(f^2 - \tilde{f}^2)g\|^2 = \int (f^2 - \tilde{f}^2)^2 g^2 \, d\mu \leq M^2 \|g\|^2 \leq M^2 \] (5–21)
and hence from Equation 5–10,
\[ \|A_2\|_{op} \leq M = \sup\{|f^2 - \tilde{f}^2|\}. \] (5–22)

Since $\|L\|_{op} \leq \|A_1\|_{op}\|A_2\|_{op}$, from Equations 5–20 and 5–22, we observe that
\[ c_0 = \|L\|_{op} \leq \frac{\sup\{|f^2 - \tilde{f}^2|\}}{\tilde{f}^2}. \] (5–23)

It is worth commenting that the bound for $c_0$ is independent of $h$. So, if we guarantee that $\frac{\sup\{|f^2 - \tilde{f}^2|\}}{\tilde{f}^2} < 1$, the geometric series approximation for $(1 + L)^{-1}$ (Equation 5–11) converges for all values of $h$.

### 5.2 Deriving a Bound for the Convergence of the Perturbation Series

Interestingly, for any positive, upper bounded forcing function $f$ bounded away from zero, i.e. $f(X) > \epsilon$ for some $\epsilon > 0^1$, by defining $\tilde{f} = \sup\{f(X)\}$, we observe that $|f^2 - \tilde{f}^2| < \tilde{f}^2$. From Equation 5–23, we immediately see that $c_0 < 1$. This proves the existence of $\tilde{f}$ for which the geometric series approximation (Equation 5–11) is always guaranteed to converge for any positive bounded forcing function $f$ bounded away from zero. The choice of $\tilde{f}$ can then be made prudently by defining it to be the value that minimizes
\[ F(\tilde{f}) = \frac{\sup\{|f^2 - \tilde{f}^2|\}}{\tilde{f}^2}. \] (5–24)

---

\(^1\) If $f(X) = 0$, then the velocity $\nu(X) = \frac{1}{\tilde{f}(X)}$ becomes $\infty$ at $X$. Hence it is reasonable to assume $f(X) > 0$. 

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This in turn minimizes the operator norm \( c_0 \), thereby providing a better geometric series approximation for the inverse (Equation 5–11).

Let \( f_{\min} = \inf \{ f(X) \} \) and let \( f_{\max} = \sup \{ f(X) \} \). We now show that \( F(\tilde{\tau}) \) attains its minimum at

\[
\tilde{\tau} = \nu = \sqrt{\frac{f_{\min}^2 + f_{\max}^2}{2}}. \tag{5–25}
\]

Case(i): If \( \tilde{\tau} < \nu \), then \( \sup \{|f^2 - \tilde{\tau}^2|\} = f_{\max}^2 - \tilde{\tau}^2 \). Clearly,

\[
\frac{f_{\max}^2 - \tilde{\tau}^2}{f^2} > \frac{f_{\max}^2 - \nu^2}{\nu^2}. \tag{5–26}
\]

Case(ii): If \( \tilde{\tau} > \nu \), then \( \sup \{|f^2 - \tilde{\tau}^2|\} = \tilde{\tau}^2 - f_{\min}^2 \). It follows that

\[
\frac{\tilde{\tau}^2 - f_{\min}^2}{\tilde{\tau}^2} = 1 - \frac{f_{\min}^2}{\tilde{\tau}^2} > 1 - \frac{f_{\min}^2}{\nu^2}. \tag{5–27}
\]

We therefore see that \( \tilde{\tau} = \nu = \sqrt{\frac{f_{\min}^2 + f_{\max}^2}{2}} \) is the optimal value.

Using the above approximation for \((1 + L)^{-1}\) from Equation 5–11 and the definition of \( L \) from Equation 5–2, we obtain the solution for \( \phi \) as

\[
\phi = \phi_0 - \phi_1 + \phi_2 - \phi_3 + \ldots + (-1)^T \phi_T \tag{5–28}
\]

where \( \phi_i \) satisfies the recurrence relation

\[
(-\hbar^2 \nabla^2 + \tilde{\tau}^2)\phi_i = (f^2 - \tilde{\tau}^2)\phi_{i-1}, \quad \forall i \in \{1, 2, \ldots, T\}. \tag{5–29}
\]

Observe that Equation 5–29 is an inhomogeneous, screened Poisson equation with a constant forcing function \( \tilde{\tau} \). Following a Green’s function approach \([2]\), each \( \phi_i \) can be obtained by convolution

\[
\phi_i = G \ast [(f^2 - \tilde{\tau}^2)\phi_{i-1}] \tag{5–30}
\]

where \( G \) is given by Equations 3–6, 3–7 or 3–8 depending upon the spatial dimension.

Once the \( \phi_i \)'s are computed, the wave function \( \phi \) can then be determined using the approximation (Equation 5–28). The solution for the eikonal equation can be recovered.
using the Equation 2–51. Notice that if \( f = \tilde{f} \) everywhere, then all \( \phi_i \)'s except \( \phi_0 \) is identically equal to zero and we get \( \phi = \phi_0 \) as described in the Chapter 3.

5.3 Efficient Computation of the Wave Function

In this section, we provide numerical techniques for efficiently computing the wave function \( \phi \). As described in Chapter 3, in order to obtain the desired solution for \( \phi_0 \) computationally, we must replace the \( \delta \) function by the Kronecker delta function

\[
\delta_{\text{kron}}(X) = \begin{cases} 
1 & \text{if } X = Y_k; \\
0 & \text{otherwise}
\end{cases}
\]

that takes 1 at the point-set locations (\( \{ Y_k \} \)) and 0 at other grid locations. Then \( \phi_0 \) can be exactly computed at the grid locations by the discrete convolution of \( \tilde{G} \) (setting \( C = 1 \)) with the Kronecker-delta function.

To compute \( \phi_i \), we replace each of the convolutions in Equation 5–30 with the discrete convolution between the functions computed at the \( N \) grid locations. As discrete convolution can be done using Fast Fourier Transforms, the values of each \( \phi_i \) at the \( N \) grid locations can be efficiently computed in \( O(N \log N) \) making use of the values of \( \phi_{i-1} \) determined at the earlier step. Thus, the overall time complexity to compute the approximate \( \phi \) using the first few \( T + 1 \) terms is then \( O(TN \log N) \). Taking the logarithm of \( \phi \) then provides an approximate solution to the eikonal equation. The algorithm is adumbrated in Table 5-1.

We would like to emphasize that the number of terms (\( T \)) used in the geometric series approximation of \( (1 + L)^{-1} \) in Equation 5–11 is independent of \( N \). Using more terms only improves the approximation of this truncated geometric series as shown in the experimental section. From Equation 5–12, it is evident that the error incurred due to this approximation converges to zero exponentially in \( T \) and hence even with a small value of \( T \), we should be able to achieve good accuracy.
Table 5-1. Algorithm for the approximate solution to the eikonal equation

1. Compute the function \( \tilde{G}(X) = \exp \left( \frac{-r\|X\|}{h} \right) \) at the grid locations.
2. Define the function \( \delta_{\text{kron}}(X) \) which takes the value 1 at the point-set locations and 0 at other grid locations.
3. Compute the FFT of \( \tilde{G} \) and \( \delta_{\text{kron}} \), namely \( \tilde{G}_{\text{FFT}}(U) \) and \( \delta_{\text{FFT}}(U) \) respectively.
4. Compute the function \( H(U) = \tilde{G}_{\text{FFT}}(U)\delta_{\text{FFT}}(U) \).
5. Compute the inverse FFT of \( H \) to obtain \( \phi_0(X) \) at the grid locations.
6. Initialize \( \phi(X) \) to \( \phi_0(X) \).
7. Consider the Green’s function \( G \) corresponding to the spatial dimension and compute its FFT, namely \( G_{\text{FFT}}(U) \).
8. For \( i = 1 \) to \( T \) do
   9. Define \( P(X) = \left[ f^2(X) - \tilde{r}^2 \right] \phi_{i-1}(X) \).
   10. Compute the FFT of \( P \) namely \( P_{\text{FFT}}(U) \).
   11. Compute the function \( H(U) = G_{\text{FFT}}(U)P_{\text{FFT}}(U) \).
   12. Compute the inverse FFT of \( H \) and multiply it with the grid width area/volume to compute \( \phi_i(X) \) at the grid locations.
   13. Update \( \phi(X) = \phi(X) + (-1)^i\phi_i(X) \).
   14. End
15. Take the logarithm of \( \phi(X) \) and multiply it by \( (-h) \) to get the approximate solution for the eikonal equation at the grid locations.

5.3.1 Numerical Issues

In principle, we should be able to apply our technique at very small values of \( h \) and obtain highly accurate results. But we noticed that a na""ive double precision-based implementation tends to deteriorate for \( h \) values very close to zero. This is due to the fact that at small values of \( h \) (and also at large values of \( \tilde{r} \) ), \( \exp \left( \frac{-r\|X\|}{h} \right) \) drops off very quickly and hence for grid locations which are far away from the point-set, the convolution done using FFT may not be accurate. To this end, we turned to the GNU MPFR multiple-precision arithmetic library which provides arbitrary precision arithmetic with correct rounding [20]. MPFR is based on the GNU multiple-precision library (GMP) [45]. It enabled us to run our technique at very small values of \( h \) giving highly accurate results. We corroborate our claim and demonstrate the usefulness of our method with the set of experiments described in the subsequent section.
5.3.2 Exact Computational Complexity

More the number of precision bits $p$ used in the GNU MPFR library, better is the accuracy of our technique, as the error incurred in the floating point operations can be bounded by $O(2^{-p})$. But using more bits has an adverse effect of slowing down the running time. The $O(N \log N)$ time complexity of the FFT algorithm [14] for an $O(N)$ length sequence takes into account only the number of floating-point operations involved, barring any numerical accuracy. The accuracy of the FFT algorithm and our technique entirely depends on the number of precision bits used for computing elementary functions like $\exp$, $\log$, $\sin$ and $\cos$ and hence should be taken into account while calculating the time complexity of our algorithm. If $p$ precision bits are used, the time complexity for computing these elementary functions can be shown to be $O(M(p) \log p)$ [8, 39, 43], where $M(p)$ is the computational complexity of multiplying two $p$-digit numbers. The Schönhage-Strassen algorithm [40] gives an asymptotic upper bound on the time complexity for multiplying two $p$-digit numbers. The run-time bit complexity is $M(p) = O(p \log p \log \log p)$. Then taking these $p$ precision bits into account, the time complexity of our algorithm for computing $S^*$ at the given $N$ grid locations, using the first $T + 1$ terms in the geometric series approximation of $\phi$ (Equation 5–28), is $O(TN \log(N)p(\log p)^2 \log(\log p))$ bit-wise operations.
CHAPTER 6
GRADIENT DENSITY ESTIMATION IN ONE DIMENSION

This chapter is focussed on using the phase relationship between the Schrödinger wave equation $\phi$ and the Hamilton-Jacobi scalar field $S$ to relate the density of the gradient of $S$ with the power spectrum of the wave function in one dimension.

6.1 Motivation from Quantum Mechanics: The Correspondence Principle

The rules imposed by quantum mechanics has been very successful in describing microscopic objects like molecules, atoms and subatomic particles like electrons. But the world of macroscopic objects are largely governed by classical mechanics say for example Newton’s laws of motion. If quantum theory is assumed to be more fundamental than its classical counterpart and should be also be capable of explaining macroscopic phenomenon, then there should be a limit where the laws of quantum mechanics become close to the laws of classical mechanics. The conditions under which the quantum and classical laws agree is called the correspondence limit or the classical limit. This principle was formulated by Bohr in early 1920s and roughly states that classical and quantum physics should give the same answer when the system becomes large. It is assumed that as $\hbar \to 0$, the laws of quantum mechanics naturally gives rise to the laws of classical mechanics, conspicuous in the Feynman’s path integral derivation of the Schrödinger wave equation [11], where the transitional amplitude or the short-time propagator $K$ is assumed to be the exponent of $\left\{ \frac{iS^*}{\hbar} \right\}$, where $S^*$ represents the classical physical action of the system (see Section 2.2.1). Hence as $\hbar \to 0$, we can expect that the wavefunction of a particle will behave like

$$\psi(X, t) \approx \alpha \exp \left\{ \frac{i}{\hbar} S^*(X, t) \right\}, \alpha = \text{constant.} \quad \text{(6–1)}$$

If $\hbar \to 0$, the exponent in Equation 6–1 becomes rapidly oscillating and then the trajectory of the particle is defined by the minimum of the action $S^*$ as in the case of the classical mechanics.
6.2 Phase Relationship Between $\phi$ and $S$

In Section 2.2.2, when we related the time-independent Schrödinger wave $\phi$ and the Hamilton’s characteristic function $S$ [22] (refer Section 2.1 through the exponent, specifically $\phi(X) = \exp(-\frac{S(X)}{\hbar})$, we showed that when $\phi$ satisfies Equation 2–44, $S$ asymptotically satisfies the eikonal equation (Equation 1–1) as $\hbar \to 0$. Recall that in deriving the equation for $\phi$ we considered the negative values for the energy $E$, namely $E = \frac{-1}{2}$, for which the differential equation satisfied by the wave function $\phi$ (Equation 2–44) had generalized functions (distributions) as solutions, which were real-valued functions. We also briefly mentioned that when $E$ is positive, for which solutions of $\phi$ are complex-valued, by relating $\phi$ and $S$ through the phase as in Equation 6–1, specifically

$$\phi(X) = \exp \left\{ \frac{i}{\hbar} S(X) \right\},$$

(6–2)

as one finds in the WKB approximation for the eikonal equation [35], $S$ can be shown to satisfy the eikonal equation in the limit as $\hbar \to 0$.

So far we ignored this phase relationship between $\phi$ and $S$. But to our amazement we observed that, the power spectrum [7] of $\phi$ in Equation 6–2 has an haunting similarity to the density of gradients of $S$. In other words the squared magnitude of the Fourier transform of the wave function is approximately equal to the density function of the gradient of $S$ with the approximation becoming increasingly exact as $\hbar \to 0$. The gradients of $S$ corresponds to the classical momentum of a particle [22]. In the parlance of quantum mechanics, the magnitude square of the wave function expressed either in its position or momentum basis corresponds to its position or momentum density respectively. Since these representations (either in the position or momentum basis) are simply the (suitably scaled) Fourier transforms of each other, the magnitude square of the Fourier transform of the wave function expressed in its position basis, is its quantum momentum density [24]. Below we rigorously show that the classical momentum density...
can be expressed as a limiting case (as $\hbar \to 0$) of the quantum momentum density, in complete agreement with the correspondence principle.

### 6.3 Density Function for the Gradients

The current chapter restricts itself with estimating the density of gradients of a thrice differentiable $S$ defined on a bounded set $\Omega$ in one dimension. The next few lines places our notion of the gradient density on a firm footing.

The probability density function of the gradients can be obtained via a random variable transformation of a uniformly distributed random variable [6] and as illustrated in [37]. Specifically, let $S : \Omega \to \mathbb{R}$ denote a thrice differentiable function defined on a closed bounded interval $\Omega = [b_1, b_2]$. Let $S'$ denote its derivative. Let $X$ denote a uniformly distributed random variable defined on $\Omega$. After restricting $S'$ to be a continuous function, define a new random variable $Y = S'(X)$. In other words, we perform a random variable transformation using $S'$ on $X$ to obtain the new random variable $Y$. The density of the random variable $Y$ then represents the density of the gradients $S'$.

In the current chapter, we provide a simple Fourier transform based technique to determine the density of $Y$. Our method computes the gradient density directly from the function $S$, circumventing the need to compute its derivative $S'$. The approach is based on expressing the function $S$ as the phase of a wave function $\phi$, specifically $\phi(x) = \exp \left( \frac{iS(x)}{\hbar} \right)$ for small values of $\hbar$ and then considering the normalized power spectrum—magnitude squared of the Fourier transform of $\phi$ [7]. Using the stationary phase approximation—a well known technique in asymptotic analysis—we show that in the limiting case as $\hbar \to 0$, the power spectrum of $\phi$ exactly matches the density of $Y$ and hence can serve as its density estimator at small, non-zero values of $\hbar$. This relationship also has strong connotations to the correspondence principle (Section 6.1) where the classical momentum density of the random variable $Y$ is expressed as a limiting case of its corresponding quantum momentum density.
6.4 Existence of the Density Function

As stated above, the density function for the gradients of \( S \) (denoted by \( Y \)) can be obtained via a random variable transformation of a uniformly distributed random variable \( X \) using the derivative \( S' \) as the transformation function, namely, \( Y = S'(X) \). We assume that \( S \) is thrice differentiable on a closed, bounded interval \( \Omega = [b_1, b_2] \) (with length \( L = b_2 - b_1 \)) and has a non-vanishing second derivative almost everywhere on \( \Omega \), i.e.

\[
\mu \left( \{ x : S''(x) = 0 \} \right) = 0,
\tag{6–3}
\]

where \( \mu \) denotes the Lebesgue measure. The assumption in Equation 6–3 is made in order to ensure that the density function of \( Y \) exists almost everywhere. This is further clarified in Lemma 3 below.

Define the following sets:

\[
\begin{align*}
\mathcal{B} & \equiv \{ x : S''(x) = 0 \}, \\
\mathcal{C} & \equiv \{ S'(x) : x \in \mathcal{B} \} \cup \{ S'(b_1), S'(b_2) \}, \text{ and} \\
\mathcal{A}_u & \equiv \{ x : S'(x) = u \}.
\end{align*}
\tag{6–4}
\]

Here, \( S'(b_1) = \lim_{x \to b_1^+} S'(x) \) and \( S'(b_2) = \lim_{x \to b_2^-} S'(x) \). The higher derivatives of \( S \) at the end points \( b_1, b_2 \) are also defined along similar lines using one-sided limits. The main purpose of defining these one-sided limits is to exactly determine the set \( \mathcal{C} \) where the density of \( Y \) is not defined. Since \( \mu(\mathcal{B}) = 0 \), we also have \( \mu(\mathcal{C}) = 0 \).

**Lemma 1** (Finiteness Lemma). \( \mathcal{A}_u \) is finite for every \( u \notin \mathcal{C} \).

**Proof.** We prove the result by contradiction. Firstly observe that \( \mathcal{A}_u \) is a subset of the compact set \( \Omega \). If \( \mathcal{A}_u \) is not finite, then by theorem (2.37) in [38], \( \mathcal{A}_u \) has a limit point \( x_0 \in \Omega \). Consider a sequence \( \{ x_n \}_{n=1}^\infty \), with each \( x_n \in \mathcal{A}_u \), converging to \( x_0 \). Since \( S'(x_n) = u, \forall n \), from the continuity of \( S' \) we get \( S'(x_0) = u \) and hence \( x_0 \in \mathcal{A}_u \). Then,

\[
\lim_{n \to \infty} \frac{S'(x_0) - S'(x_n)}{x_0 - x_n} = 0 = S''(x_0).
\tag{6–5}
\]
Based on the definitions given in Equation 6–4, we have $x_0 \in B$ and hence $u \in C$ resulting in a contradiction.

**Lemma 2** (Interval Lemma). For every $u \notin C$, $\exists \eta > 0$ and a closed interval $\mathcal{J}_\eta = [u - \eta, u + \eta]$, such that $\mathcal{J}_\eta \cap C$ is empty.

*Proof.* Observe that $B$ is closed because if $x_0$ is a limit point of $B$, from the continuity of $S''$ we have $S''(x_0) = 0$ and hence $x_0 \in B$. $B$ is also compact as it is a closed subset of $\Omega$. Since $S'$ is continuous, $C = S'(B) \cup \{S'(b_1), S'(b_2)\}$ is also compact and hence $\mathbb{R} - C$ is open. Then for $u \notin C$, there exists an open neighborhood $\mathcal{N}_r(u)$ for some $r > 0$ around $u$ such that $\mathcal{N}_r(u) \cap C = \emptyset$. By defining $\eta = \frac{r}{2}$, the proof is complete.

**Lemma 3** (Density Lemma). The probability density of $Y$ on $\mathbb{R} - C$ exists and is given by

$$P(u_0) = \frac{1}{L} \sum_{k=1}^{N(u_0)} \frac{1}{|S''(x_k)|},$$

(6–6)

where the summation is over $A_{u_0}$ (which is the finite set of locations $x_k \in \Omega$ where $S'(x_k) = u_0$ as per Lemma 1, with $|A_{u_0}| = N(u_0)$).

*Proof.* Since the random variable $X$ is assumed to have a uniform distribution on $\Omega$, its density is given by $f_X(x) = \frac{1}{L}$ for every $x \in \Omega$. Recall that the random variable $Y$ is obtained via a random variable transformation from $X$, using the function $S'$. Hence, its density function exists on $\mathbb{R} - C$—where we have banished the image (under $S'$) of the measure zero set of points where $S''$ vanishes—and is given by Equation 6–6. The reader may refer to [6] for a detailed explanation.

### 6.5 Equivalence of the Gradient Density and the Power Spectrum

We now prove the main result that relates the normalized power spectrum of $\exp \left( \frac{iS(x)}{\hbar} \right)$ (in the limit as $\hbar \to 0$) with the probability density of the random variable $Y$ (denoted by $P$).
Let $L = b_2 - b_1$. Define a function $F : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{C}$ as
\[
F(u, \hbar) \equiv \frac{1}{\sqrt{2\pi \hbar L}} \int_{b_1}^{b_2} \exp \left( \frac{iS(x)}{\hbar} \right) \exp \left( -\frac{iu x}{\hbar} \right) \, dx. \tag{6-7}
\]

For a fixed value of $\hbar$, define a function $F_\hbar : \mathbb{R} \to \mathbb{C}$ as
\[
F_\hbar(u) \equiv F(u, \hbar). \tag{6-8}
\]

Observe that $F_\hbar$ is closely related to the Fourier transform of $\exp \left( \frac{iS(x)}{\hbar} \right)$. The scale factor $\frac{1}{\sqrt{2\pi \hbar L}}$ is the normalizing term such that the $L_2$ norm of $F_\hbar$ is one as seen in the following lemma.

**Lemma 4.** With $F_\hbar$ defined as above, $F_\hbar \in L^2(\mathbb{R})$ and $\|F_\hbar\| = 1$.

**Proof.** Define a function $H(x)$ by
\[
H(x) \equiv \begin{cases} 
1 & \text{if } x \in [b_1, b_2]; \\
0 & \text{otherwise}
\end{cases}
\]

Let $f(x) = H(x) \exp \left( \frac{iS(x)}{\hbar} \right)$. Then,
\[
F_\hbar(u) = \frac{1}{\sqrt{2\pi \hbar L}} \int_{-\infty}^{\infty} f(x) \exp \left( -\frac{iu x}{\hbar} \right) \, dx. \tag{6-9}
\]

Let $\frac{u}{\hbar} = \nu$ and $G(\nu) = F_\hbar(\nu \hbar)$. Then,
\[
\sqrt{\hbar L} G(\nu) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp(-i\nu x) \, dx. \tag{6-10}
\]

Since $f$ is $L^1$ integrable, by Parseval's theorem [7] we have,
\[
\int_{-\infty}^{\infty} |f(x)|^2 \, dx = \int_{-\infty}^{\infty} |\sqrt{\hbar L} G(\nu)|^2 \, d\nu = \hbar L \int_{-\infty}^{\infty} |F_\hbar(\nu \hbar)|^2 \, d\nu. \tag{6-11}
\]

By letting $u = \nu \hbar$ and observing that
\[
\int_{-\infty}^{\infty} |f(x)|^2 \, dx = \int_{b_1}^{b_2} \left| \exp \left( \frac{iS(x)}{\hbar} \right) \right|^2 \, dx = L, \tag{6-12}
\]
we get
\[ L \int_{-\infty}^{\infty} |F_h(u)|^2 \, du = L. \] (6–13)

Hence
\[ \int_{-\infty}^{\infty} |F_h(u)|^2 \, du = 1, \] (6–14)

which completes the proof. □

Define a function \( P_h : \mathbb{R} - \mathcal{C} \to \mathbb{R}^+ \) as
\[ P_h(u) \equiv |F_h(u)|^2 = F_h(u)\overline{F_h(u)}. \] (6–15)

By definition, \( P_h \geq 0 \). Since \( \mu(\mathcal{C}) = 0 \), from Lemma 4, \( \int_{-\infty}^{\infty} P_h(u) \, du = 1 \). Hence, treating \( P_h(u) \) as a density function, we have the following theorem statement.

**Theorem 6.1.** If \( P \) and \( P_h \) are defined as above, then
\[ \lim_{\alpha \to 0} \lim_{h \to 0} \int_{u_0}^{u_0 + \alpha} P_h(u) \, du = P(u_0), \ \forall u_0 \notin \mathcal{C}. \] (6–16)

Before embarking on the proof, we would like to emphasize that the ordering of the limits and the integral as given in the theorem statement is crucial and cannot be arbitrarily interchanged. To press this point home, we show below that after solving for \( P_h \), the limit \( \lim_{h \to 0} P_h \) does not exist. Hence, the order of the integral followed by the limit \( h \to 0 \) cannot be interchanged. Furthermore, when we swap the limits between \( \alpha \) and \( h \), we get
\[ \lim_{h \to 0} \lim_{\alpha \to 0} \int_{u_0}^{u_0 + \alpha} P_h(u) \, du = \lim_{\alpha \to 0} \lim_{h \to 0} P_h(u_0) \] (6–17)

which does not exist. Hence, the theorem statement can be valid only for the specified sequence of limits and the integral.

**6.5.1 Brief Exposition of the Result**

To understand the result in simpler terms, let us reconsider the definition of the scaled Fourier transform given in Equation 6–7. The first exponential \( \exp \left( \frac{iS}{h} \right) \) is a varying complex sinusoid, whereas the second exponential \( \exp \left( \frac{-iu\alpha}{h} \right) \) is a fixed complex sinusoid
at frequency $\frac{u}{h}$. When we multiply these two complex exponentials, at low values of $h$, the two sinusoids are usually not in sync and tend to cancel each other out. However, around the locations where $S'(x) = u$, the two sinusoids are in perfect sync (as the combined exponent is stationary) with the approximate duration of this resonance depending on $S''(x)$. The value of the integral in Equation 6–7 can be approximated via the stationary phase approximation [31] as

$$F_h(u) \approx \frac{1}{\sqrt{L}} \exp \left( \pm \frac{i \pi}{4} \right) \sum_{k=1}^{N(u)} \exp \left\{ \frac{i}{h} (S(x_k) - ux_k) \right\} \frac{1}{\sqrt{S''(x_k)}}$$  \hspace{1cm} (6–18)

where $N(u) = |A_u|$. The approximation is increasingly tight as $h \to 0$. The squared Fourier transform ($P_h$) gives us the required result except for the cross phase factors $S(x_k) - S(x_l) - u(x_k - x_l)$ obtained as a byproduct of two or more remote locations $x_k$ and $x_l$ indexing into the same frequency bin $u$, i.e, $x_k \neq x_l$, but $S'(x_k) = S'(x_l) = u$. Integrating the squared Fourier transform over a small frequency range $[u, u + \alpha]$ removes these cross phase factors and we obtain the desired result.

6.5.2 Formal Proof

We shall now provide the proof by considering different cases.

Proof. case (i): Let us consider the case in which no stationary points exist for the given $u_0$, i.e, there is no $x \in \Omega$ for which $S'(x) = u_0$. Let $t(x) = S(x) - u_0 x$. Then, $t'(x)$ is of constant sign in $[b_1, b_2]$ and hence $t(x)$ is strictly monotonic. Defining $\nu = t(x)$, we have from Equation 6–7,

$$F_h(u_0) = \frac{1}{\sqrt{2\pi h L}} \int_{t(b_1)}^{t(b_2)} \exp \left( \frac{iv}{h} \right) g(v) dv.$$  \hspace{1cm} (6–19)

Here, $g(v) = \frac{1}{v(t(x))}$ where $x = t^{-1}(v)$. Integrating by parts, we get

$$F_h(u_0) \sqrt{2\pi h L} = \frac{h}{i} \left[ \exp \left( \frac{it(b_2)}{h} \right) g(t(b_2)) - \exp \left( \frac{it(b_1)}{h} \right) g(t(b_1)) \right]$$

$$- \frac{h}{i} \int_{t(b_1)}^{t(b_2)} \exp \left( \frac{iv}{h} \right) g'(v) dv.$$  \hspace{1cm} (6–20)
Then
\[
|F_h(u_0)| \sqrt{2\pi h L} \leq h \left( \frac{1}{|S'(b_2) - u_0|} + \frac{1}{|S'(b_1) - u_0|} + \int_{t(b_1)}^{t(b_2)} |g'(v)| \, dv \right).
\] (6–21)

Hence, \( |F_h(u_0)| \leq \gamma(u_0) \sqrt{h} \), where \( \gamma(u_0) > 0 \) is some continuous function of \( u_0 \). Then
\[
P_h(u_0) \leq \gamma^2(u_0) h.
\]
Since \( S'(x) \) is continuous and \( u_0 \notin C \), we can find a \( \rho > 0 \) such that for every \( u \in [u_0 - \rho, u_0 + \rho] \), no stationary points exist. The value \( \rho \) can also be chosen appropriately such that \( [u_0 - \rho, u_0 + \rho] \cap C = \emptyset \). If \( |\alpha| < \rho \), then
\[
\lim_{h \to 0} \int_{u_0}^{u_0 + \alpha} P_h(u) \, du = 0.
\] (6–22)

Furthermore, from Equation 6–6 we have \( P(u_0) = 0 \). The result immediately follows.

Case (ii): We now consider the case where stationary points exist. Since we are interested only in the situation as \( h \to 0 \), the stationary phase method in [31, 32] can be used to obtain a good approximation for \( F_h(u_0) \) defined in Equations 6–7 and 7–13. The phase term in this function, \( \frac{S(x) - u_0 x}{h} \), is stationary only when \( S'(x) = u_0 \). Consider the set \( A_{u_0} \) defined in Equation 6–4. Since it is finite by Lemma 1, let \( A_{u_0} = \{ x_1, x_2, \ldots, x_{N(u_0)} \} \) with \( x_k < x_{k+1}, \forall k \). We break \( \Omega \) into disjoint intervals such that each interval has utmost one stationary point. To this end, consider numbers \( \{ c_1, c_2, \ldots, c_{N(u_0)+1} \} \) such that
\[
b_1 < c_1 < x_1, x_k < c_{k+1} < x_{k+1} \text{ and } x_{N(u_0)} < c_{N(u_0)+1} < b_2.\]
Let \( t(x) = S(x) - u_0 x \). Then
\[
F_h(u_0) \sqrt{2\pi h L} = G_1 + G_2 + \sum_{k=1}^{N(u_0)} (K_k + \tilde{K}_k)
\] (6–23)
where
\[
G_1 = \int_{b_1}^{c_1} \exp \left( \frac{it(x)}{h} \right) \, dx,
\]
\[
G_2 = \int_{c_{N(u_0)+1}}^{b_2} \exp \left( \frac{it(x)}{h} \right) \, dx,
\]
\[
K_k = \int_{c_k}^{x_k} \exp \left( \frac{it(x)}{h} \right) \, dx, \text{ and}
\]
\[
\tilde{K}_k = \int_{x_k}^{c_{k+1}} \exp \left( \frac{it(x)}{h} \right) \, dx.
\] (6–24)
Note that the integrals $G_1$ and $G_2$ do not have any stationary points. From case (i) above, we get
\[ G_1 + G_2 = \epsilon_1(u_0, h) = O(h) \]  
(6–25)
as $h \to 0$. Furthermore, $\epsilon_1(u_0, h) \leq \gamma_2(u_0) h$, where $\gamma_2(u_0) > 0$ is a continuous function of $u_0$. In order to evaluate $K_k$ and $\tilde{K}_k$, observe that when we expand the phase term up to second order, $t(x) - t(x_k) \to Q(x_k)(x - x_k)^2$ as $x \to x_k$, where $Q(x_k) = \frac{S''(x_k)}{2}$. Furthermore, in the open intervals $(c_k, x_k)$ and $(x_k, c_{k+1})$, $t'(x) = S'(x) - u_0$ is continuous and is of constant sign. From theorem (13.1) in [31], we get
\[ \tilde{K}_k = K_k = \frac{1}{2} \exp \left( \pm \frac{i\pi}{4} \right) \Gamma \left( \frac{1}{2} \right) \exp \left( \frac{it(x_k)}{h} \right) \sqrt{\frac{2h}{|S''(x_k)|}} + \epsilon_2(u_0, h). \]  
(6–26)
From lemma (12.3) in [31], it can be verified that $\epsilon_2(u_0, h) = o(\sqrt{h})$ as $h \to 0$ and can also be uniformly bounded by a function of $u_0$ (independent of $h$) for small values of $h$.

In Equation 6–26, $\Gamma$ is the Gamma function and the sign in the phase term depends on whether $S''(x_k) > 0$ or $S''(x_k) < 0$. Plugging the values of these integrals in Equation 6–23 and noting that $\Gamma \left( \frac{1}{2} \right) = \sqrt{\pi}$, we get
\[ F_h(u_0) \sqrt{2\pi h L} = \sum_{k=1}^{N(u_0)} \exp \left( \frac{i}{h} [S(x_k) - u_0 x_k] \right) \sqrt{\frac{2\pi h}{|S''(x_k)|}} \exp \left( \pm \frac{i\pi}{4} \right) + \epsilon_1(u_0, h) + \epsilon_2(u_0, h). \]  
(6–27)
Hence,
\[ F_h(u_0) = \frac{1}{\sqrt{L}} \sum_{k=1}^{N(u_0)} \frac{\exp \left( \frac{i}{h} [S(x_k) - u_0 x_k] \right)}{\sqrt{|S''(x_k)|}} \exp \left( \pm \frac{i\pi}{4} \right) \]  
(6–28)
\[ + \epsilon_3(u_0, h), \]  
(6–29)
where $\epsilon_3(u_0, h) = \frac{\epsilon_1(u_0, h) + \epsilon_2(u_0, h)}{\sqrt{2\pi h L}} = o(1)$ as $h \to 0$. 

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From the definition of $P_h(u)$ in Equation 7–35, we have

$$
\begin{align*}
P_h(u_0) & = \frac{1}{L} \sum_{k=1}^{N(u_0)} \frac{1}{|S''(x_k)|} \\
& + \frac{1}{L} \sum_{k=1}^{N(u_0)} \sum_{l=1; l\neq k}^{N(u_0)} \frac{\cos \left( \frac{i}{\hbar} [S(x_k) - S(\xi_l) - u_0(x_k - \xi_l)] + \theta(x_k, \xi_l) \right)}{|S''(x_k)|^{3/2} |S''(\xi_l)|^{3/2}} \\
& + \epsilon_4(u_0, \hbar),
\end{align*}
$$

(6–30)

where $\epsilon_4(u_0, \hbar)$ includes both the magnitude square of $\epsilon_3(u_0, \hbar)$ and the cross product between the main (first) term in Equation 6–28 and $\epsilon_3(u_0, \hbar)$. Notice that the main term in Equation 6–28 can be bounded by a function of $u_0$ independent of $\hbar$ as

$$
\exp \left( \frac{i}{\hbar} [S(x_k) - u_0 x_k] \right) = 1, \forall \hbar
$$

(6–31)

and $S''(x_k) \neq 0, \forall k$. Since $\epsilon_3(u_0, \hbar) = O(1)$, we get $\epsilon_4(u_0, \hbar) = O(1)$ as $\hbar \to 0$. Additionally, $\theta(x_k, \xi_l) = 0$, $\pi/2$ (or) $-\pi/2$ and $\theta(x_l, x_k) = -\theta(x_k, x_l)$.

Notice that the first term in Equation 6–30 exactly matches the expression for $P(u_0)$ as seen from Lemma 3. But, since $\lim_{\hbar \to 0} \cos \left( \frac{i}{\hbar} \right)$ is not defined, $\lim_{\hbar \to 0} P_h(u_0)$ does not exist and hence the cross cosine terms do not vanish when we take the limit. We now show that integrating $P_h(u)$ over a small non-zero interval $[u_0, u_0 + \alpha]$ and then taking the limit with respect to $\hbar$ (followed by the limit with respect to $\alpha$) does yield the density of $\mathcal{Y}$.

From Lemmas 1 and 2, we see that for a given $a \in \mathcal{A}_{u_0}$, when $u$ is varied over the interval $\mathcal{J}_\eta = [u_0 - \eta, u_0 + \eta]$, the inverse function $(S')^{-1}(u)$ is well defined with $(S')^{-1}(u) \in \mathcal{N}_a$, where $\mathcal{N}_a$ is some small neighborhood around $a$. For each $a \in \mathcal{A}_{u_0}$, define the inverse function $(S'_a)^{-1}(u) : \mathcal{J}_\eta \to \mathcal{N}_a$ as

$$
(S'_a)^{-1}(u) = x \text{ iff } u = S'(x) \text{ and } x \in \mathcal{N}_a.
$$

(6–32)

When we move from $P_h(u_0)$ to $P_h(u)$, the locations $x_k$ and $\xi_l$ in Equation 6–30 become functions of $u$. Using the inverse functions defined in Equation 6–32 and defining $a_k \equiv x_k(u_0)$ and $a_l \equiv x_l(u_0)$, $x_k(u) = (S'_{a_k})^{-1}(u)$ and $\xi_l(u) = (S'_{a_l})^{-1}(u)$ for $u \in \mathcal{J}_\eta$. Define
the functions \( p_{kl}(u) \) and \( q_{kl}(u) \) over \( J_\eta \) as

\[
\begin{align*}
p_{kl}(u) &\equiv S(x_k(u)) - S(x_i(u)) - u(x_k(u) - x_i(u)), \quad \text{and} \\
q_{kl}(u) &\equiv \frac{1}{|S''(x_k(u))|^\frac{1}{2} |S''(x_i(u))|^\frac{1}{2}}. 
\end{align*}
\]

(6–33) (6–34)

Observe that

\[
p_{0,kl}(u) = S(x_k(u)) x_0(k(u)) x_0(l(u)) x_k(u) x_l(u).
\]

(6–35)

as \( u = S'(x_k(u)) = S'(x_i(u)) \). In particular, if \( x_i(u_0) > x_k(u_0) \), then \( x_i(u) > x_k(u) \) and vice versa. Hence, \( p_{kl}(u) \) never vanishes and is also of constant sign over \( J_\eta \). Then, it follows that \( p_{kl}(u) \) is strictly monotonic and specifically bijective on \( J_\eta \). We will use this result in the subsequent steps.

Now, let \(|\alpha| < \eta\). Since the additional error term \( \epsilon_u(u_0,h) \) in Equation 6–30 converges to zero as \( h \to 0 \) and can also be uniformly bounded by a function of \( u_0 \) for small values of \( h \), we have

\[
\lim_{h \to 0} \int_{u_0}^{u_0+\alpha} \epsilon_u(u_0,h) du = 0. 
\]

(6–36)

Then, we get

\[
\lim_{h \to 0} \int_{u_0}^{u_0+\alpha} P_h(u) du = l_1 + l_2 
\]

(6–37)

where

\[
l_1 \equiv \frac{1}{L} \sum_{k=1}^{N(u_0)} \int_{u_0}^{u_0+\alpha} \frac{1}{|S''(x_k(u))|} du, \quad \text{and} \\
l_2 \equiv \frac{1}{L} \sum_{k=1}^{N(u_0)} \sum_{l=1, l \neq k}^{N(u_0)} \lim_{h \to 0} l_3(k,l).
\]

(6–38) (6–39)

Here, \( l_3(k,l) \) is given by

\[
l_3(k,l) \equiv \int_{u_0}^{u_0+\alpha} q_{kl}(u) \cos \left( \frac{p_{kl}(u)}{h} + \theta(x_k(u), x_i(u)) \right) du. 
\]

(6–40)
When \(|\alpha| < \eta\), the sign of \(S''(x_k(u))\) around \(x_k(u_0)\) and the sign of \(S''(x_l(u))\) around \(x_l(u_0)\) do not change over the interval \([u_0, u_0 + \alpha]\). Since \(\theta(x_k, x_l)\) depends on the sign of \(S''\), \(\theta\) is constant on \([u_0, u_0 + \alpha]\) and equals \(\theta_{kl} = \theta(x_k(u_0), x_l(u_0))\). Now, expanding the cosine term in Equation 6–40, we get

\[ I_3(k,l) = \cos(\theta_{kl}) \int_{u_0}^{u_0 + \alpha} q_{kl}(u) \cos \left( \frac{p_{kl}(u)}{h} \right) \, du \]

\[ - \sin(\theta_{kl}) \int_{u_0}^{u_0 + \alpha} q_{kl}(u) \sin \left( \frac{p_{kl}(u)}{h} \right) \, du. \]  

(6–41)

Since \(p_{kl}(u)\) is bijective, by defining \(v_{kl} = p_{kl}(u)\), we get

\[ I_3(k,l) = \cos(\theta_{kl}) I_4(k,l) - \sin(\theta_{kl}) I_5(k,l) \]  

(6–42)

where

\[ I_4(k,l) = \int_{\beta_{kl}^{(1)}}^{\beta_{kl}^{(2)}} \cos \left( \frac{v}{h} \right) g_{kl}(v) \, dv, \text{ and} \]

\[ I_5(k,l) = \int_{\beta_{kl}^{(1)}}^{\beta_{kl}^{(2)}} \sin \left( \frac{v}{h} \right) g_{kl}(v) \, dv. \]  

(6–43)

(6–44)

Here, \(\beta_{kl}^{(1)} = p_{kl}(u_0)\), \(\beta_{kl}^{(2)} = p_{kl}(u_0 + \alpha)\) and \(g_{kl}(v) = \frac{q_{kl}(u)}{p_{kl}(u)}\) where \(u = p_{kl}^{-1}(v)\).

Integrating \(I_4(k,l)\) by parts, we get

\[ I_4(k,l) = h \sin \left( \frac{\beta_{kl}^{(2)}}{h} \right) g_{kl} \left( \beta_{kl}^{(2)} \right) - h \sin \left( \frac{\beta_{kl}^{(1)}}{h} \right) g_{kl} \left( \beta_{kl}^{(1)} \right) \]

\[ - h \int_{\beta_{kl}^{(1)}}^{\beta_{kl}^{(2)}} \sin \left( \frac{v}{h} \right) g'_{kl}(v) \, dv. \]  

(6–45)

Then,

\[ |I_4(k,l)| \leq h \left( g_{kl} \left( \beta_{kl}^{(2)} \right) + g_{kl} \left( \beta_{kl}^{(1)} \right) + \int_{\beta_{kl}^{(1)}}^{\beta_{kl}^{(2)}} |g'_{kl}(v)| \, dv \right). \]  

(6–46)

It is worth mentioning that \(q_{kl}\) and hence \(g_{kl}\) are differentiable over their respective intervals as the sign of \(S''(x_k(u))S''(x_l(u))\) does not change over the interval \([u_0, u_0 + \alpha]\).

We then have \(|I_4(k,l)| \leq hM\) where \(M\) is some constant independent of \(h\). Hence,

\[ \lim_{h \to 0} I_4(k,l) = 0, \forall k, l. \]  

By a similar argument, \(\lim_{h \to 0} I_5(k,l) = 0, \forall k, l.\) From
Equations 6–39 and 6–42 we get \( l_2 = 0 \). Since

\[
\lim_{\alpha \to 0} \frac{1}{\alpha} I_1 = \frac{1}{L} \sum_{k=1}^{N(u_0)} \frac{1}{|S''(x_k)|} = P(u_0),
\]

(6–47)

the result follows.

6.5.3 Significance of the Result

Observe that the integrals

\[
I_h(u_0) = \int_{u_0}^{u_0+\alpha} P_h(u)du, \quad I(u_0) = \int_{u_0}^{u_0+\alpha} P(u)du
\]

(6–48)

give the interval measures of the density functions \( P_h \) and \( P \) respectively. Theorem 6.1 states that at small values of \( h \), both the interval measures are approximately equal, with the difference between them being \( o(1) \). Recall that by definition, \( P_h \) is the normalized power spectrum [7] of the wave function \( \phi(x) = \exp \left( \frac{iS(x)}{h} \right) \). Hence, we conclude that the power spectrum of \( \phi(x) \) can potentially serve as a density estimator for the gradients of \( S \) at small values of \( h \). The experimental results shown under Section 8.4 serve as a demonstration, anecdotally attesting to the verity of the result.
CHAPTER 7
DENSITY ESTIMATION FOR THE DISTANCE TRANSFORMS

We described in Chapter 3 that the Euclidean distance transforms satisfies the static, non-linear Hamilton-Jacobi equation

\[ \| \nabla S \| = 1. \] (7–1)

In Chapters 2 and 6 we briefly explained that when we consider positive values for the energy \( E \) in Equation 2–41 (say \( E = \frac{1}{2} \)), the aforementioned non-linear Hamilton-Jacobi equation (Equation 7–1) can be embedded in the linear Schrödinger wave equation

\[ -\hbar^2 \nabla^2 \phi = \phi, \] (7–2)

where by relating \( S \) and \( \phi \) through the phase as in Equation 6–2, \( S \) can be shown to satisfy the eikonal equation in the limit as \( \hbar \to 0 \). We call this wave function \( \phi \) satisfying the phase relation with \( S \) (Equation 6–2) as the complex wave representation (CWR) of the distance transforms.

As mentioned in Chapter 6, we observed a peculiar fact between the power spectrum (squared Fourier transform) of this wave function \( \phi \) and the density function corresponding to the gradients \( \nabla S = (S_x, S_y) \) of the distance function in two spatial dimensions. As the norm of the gradient \( \nabla S \) is defined to be 1 everywhere (refer Equation 7–1), we noticed that the Fourier transform values lies mainly on the unit circle and this behavior tightens as \( \hbar \to 0 \). In the subsequent sections using stationary phase approximations we describe an empirical discovery corroborated by theoretical analysis. We show that the squared magnitude of the Fourier transform when polled on the unit circle is approximately equal to the density function of the distance transform gradients with the approximation becoming increasingly exact as \( \hbar \to 0 \).
7.1 Density Function for the Distance Transforms

The geometry of the distance transform corresponds to a set of intersecting cones with the origins at the Voronoi centers [5]. As mentioned above, the gradients of the distance transform (which exist globally except at the cone intersections and origins) are unit vectors and satisfy Equation 7–1. Therefore the gradient density function is one-dimensional and defined over the space of orientations. The orientations are constant and unique along each ray of each cone. Its probability distribution function is given by

\[ 
F(\theta \leq \Theta \leq \theta + \Delta) \equiv \frac{1}{L} \int_\theta^{\theta + \Delta} \frac{d\theta}{\sqrt{S_x^2 + S_y^2}} dx dy \tag{7–3} 
\]

where we have expressed the orientation random variable as \( \Theta = \arctan \left( \frac{S_y}{S_x} \right) \). The probability distribution function also induces a closed-form expression for its density function as shown below.

Let \( \Omega \) denote a polygonal grid such that its boundary \( \partial \Omega \) is composed of a finite sequence of straight line segments. The reason for considering a polygonal domain and not other domains like a circular region will become clearer when we discuss Theorem 7.1. Let the set \( Y = \{ Y_k \in \mathbb{R}^2, \ k \in \{1, \ldots, K\} \} \) be the given point-set locations. Then the Euclidean distance transform at a point \( X = (x, y) \in \Omega \) is given by

\[ 
S(X) \equiv \min_k \|X - Y_k\| = \min_k \sqrt{(x - x_k)^2 + (y - y_k)^2}. \tag{7–4} 
\]

Let \( D_k \), centered at \( Y_k \), denote the \( k^{th} \) Voronoi region corresponding to the input point \( Y_k \). \( D_k \) can be represented by the cartesian product \([0, 2\pi) \times [0, R_k(\theta)]\) where \( R_k(\theta) \) is the length of the ray of the \( k^{th} \) cone at orientation \( \theta \). If a grid point \( X = (x, y) \in Y_k + D_k \), then \( S(X) = \|X - Y_k\| \). Each \( D_k \) is a convex polygon whose boundary \( \partial D_k \) is also composed of a finite sequence of straight line segments as shown in Figure 7-1.

Note that even for points that lie on the Voronoi boundary–where the radial length equals \( R_k(\theta) \)–the distance transform is well defined. The area \( L \) of the polygonal grid \( \Omega \)
is given by,

\[ L = \sum_{k=1}^{K} \int_{0}^{2\pi} \int_{0}^{R_k(\theta)} r dr d\theta = \sum_{k=1}^{K} \int_{0}^{2\pi} \frac{R_k^2(\theta)}{2} d\theta. \]  \hspace{1cm} (7–5) \]

Let \( l = \sqrt{L} \).

With the above set-up in place, by recognizing the cone geometry at each Voronoi center \( Y_k \), Equation 7–3 can be simplified as

\[ \mathcal{F}(\theta \leq \Theta \leq \theta + \Delta) \equiv \frac{1}{L} \sum_{k=1}^{K} \int_{\theta}^{\theta+\Delta} \int_{0}^{R_k(\theta)} r dr d\theta = \frac{1}{L} \sum_{k=1}^{K} \int_{\theta}^{\theta+\Delta} \frac{R_k^2(\theta)}{2} d\theta. \]  \hspace{1cm} (7–6) \]

Following this drastic simplification, we can write the closed-form expression for the density function of the unit vector distance transform gradients as

\[ P(\theta) \equiv \lim_{\Delta \to 0} \frac{\mathcal{F}(\theta \leq \Theta \leq \theta + \Delta)}{\Delta} = \frac{1}{L} \sum_{k=1}^{K} \frac{R_k^2(\theta)}{2}. \]  \hspace{1cm} (7–7) \]

Based on the expression for \( L \) in Equation 7–5 it is easy to see that

\[ \int_{0}^{2\pi} P(\theta) d\theta = 1. \]  \hspace{1cm} (7–8) \]

Since the Voronoi cells are convex polygons [5], each cell contributes exactly one conical ray to the density function on orientation. When \( S \) is treated as the Hamilton-Jacobi scalar field, \( P(\theta) \) carries an interpretation as its classical momentum density [22].

Figure 7-1. Voronoi diagram of the given \( K \) points. Each Voronoi boundary is made of straight line segments.
7.2 Properties of the Fourier Transform of CWR

Since the distance transform is not differentiable at the point-set locations \( \{ Y_k \}_{k=1}^K \) and also along the Voronoi boundaries \( \partial D_k, \forall k \) (a measure zero set in 2D), we would like to consider the region which excludes both of them. To this end, let \( 0 < \epsilon < \frac{1}{2} \) be given. Let the region \( D_k^\epsilon \) centered at \( Y_k \) be represented by the cartesian product \([0, 2\pi) \times [R_k^{(1)}(\theta), R_k^{(2)}(\theta)]\) where,

\[
R_k^{(1)}(\theta) = \epsilon R_k(\theta) \\
R_k^{(2)}(\theta) = (1 - \epsilon) R_k(\theta).
\]  

(7–9)

As before, the length of the ray at an orientation \( \theta \) in each \( D_k^\epsilon \), given by \( R_k^{(2)}(\theta) - R_k^{(1)}(\theta) \) depends on \( \theta \). Note that in the definition of \( D_k^\epsilon \) we explicitly removed the source point \( Y_k \) where the ray length \( r(\theta) = 0 \) and the boundary of the \( k^{th} \) Voronoi cell where \( r(\theta) = R_k(\theta) \).

Figure 7-2. Region that excludes both the source point and the Voronoi boundary.

Define the grid

\[
\Omega^\epsilon \equiv \bigcup_{k=1}^K Y_k + D_k^\epsilon.
\]  

(7–10)

It is worth emphasizing that \( \Omega^\epsilon \) also excludes all the source points \( \{ Y_k \}_{k=1}^K \) and the Voronoi boundaries. Its area \( L^\epsilon \) equals

\[
L^\epsilon = \sum_{k=1}^K \int_0^{2\pi} \int_{R_k^{(1)}(\theta)}^{R_k^{(2)}(\theta)} r dr d\theta = (1 - 2\epsilon) \sum_{k=1}^K \int_0^{2\pi} \frac{R_k^2(\theta)}{2} d\theta.
\]  

(7–11)

From Equation 7–5 we have \( L^\epsilon = (1 - 2\epsilon)L \) and hence \( \lim_{\epsilon \to 0} L^\epsilon = L \).
Let \( l^e = \sqrt{L^e} \). Define a function \( F^e : \mathbb{R} \times \mathbb{R} \times \mathbb{R}^+ \to \mathbb{C} \) by

\[
F^e(u, v, h) = \frac{1}{2\pi h l^e} \int_{\Omega^e} \exp \left( \frac{iS(x, y)}{h} \right) \exp \left( -i\frac{(ux + vy)}{h} \right) \, dx \, dy.
\] (7-12)

For a fixed value of \( \hbar \), define a function \( F^e_h : \mathbb{R} \times \mathbb{R} \to \mathbb{C} \) by

\[
F^e_h(u, v) = F^e(u, v, \hbar).
\] (7-13)

Note that \( F^e_h \) is closely related to the Fourier transform of the CWR, \( \phi = \exp \left( \frac{iS}{\hbar} \right) \) [7]. The scale factor \( \frac{1}{2\pi h l^e} \) is the normalizing term such that the \( L_2 \) norm of \( F^e_h \) is 1 as seen in the following lemma.

**Lemma 5.** With \( F^e_h \) defined as above, \( F^e_h \in L^2(\mathbb{R}^2) \) and \( \|F^e_h\| = 1 \).

**Proof.** Define a function \( H(x, y) \) by

\[
H(x, y) = \begin{cases} 1 & \text{if } (x, y) \in \Omega^e; \\ 0 & \text{otherwise} \end{cases}
\]

Let \( f(x, y) = H(x, y) \exp \left( \frac{iS(x, y)}{\hbar} \right) \). Then,

\[
F^e_h(u, v) = \frac{1}{2\pi h l^e} \int_{\Omega^e} f(x, y) \exp \left( -i\frac{(ux + vy)}{\hbar} \right) \, dx \, dy.
\] (7-14)

Let \( \frac{v}{\hbar} = s, \frac{v}{h} = t \) and \( G(s, t) = F^e_h(sh, th) \). Then,

\[
h^l p \, G(s, t) = \frac{1}{2\pi} \int_{\Omega^e} f(x, y) \exp(-i(sx + ty)) \, dx \, dy.
\] (7-15)

Since \( f \) is \( L^1 \) integrable, by Parseval's theorem [7] we have,

\[
\iint |f(x, y)|^2 \, dx \, dy = \iint |h^l p \, G(s, t)|^2 \, ds \, dt = (h^l)^2 \iint |F^e_h(sh, th)|^2 \, ds \, dt.
\] (7-16)

By letting \( u = sh, v = th \) and observing that

\[
\iint |f(x, y)|^2 \, dx \, dy = \iint_{\Omega^e} \left| \exp \left( \frac{iS(x, y)}{h} \right) \right|^2 \, dx \, dy = L^e,
\] (7-17)
we get
\[(l^2)^2 \int \int |F^\epsilon_h(u, v)|^2 \, du \, dv = L^\epsilon. \quad (7-18)\]

Hence
\[\int \int |F^\epsilon_h(u, v)|^2 \, du \, dv = 1, \quad (7-19)\]
which completes the proof. \(\square\)

Consider the polar representation of the spatial frequencies \((u, v)\) namely \(u = \tilde{r} \cos(\omega)\) and \(v = \tilde{r} \sin(\omega)\) where \(\tilde{r} > 0\). For \((x, y) \in Y_k + D^\epsilon_k\), let \(x - x_k = r \cos(\theta)\) and \(y - y_k = r \sin(\theta)\) with \(r \in [R^{(1)}_k(\theta), R^{(2)}_k(\theta)]\). Then Equation 7–12 can be rewritten as

\[F^\epsilon_h(\tilde{r}, \omega) = \sum_{k=1}^K C_k I_k(\tilde{r}, \omega) \quad (7-20)\]

where,

\[C_k = \exp \left( \frac{-i}{\hbar} [\tilde{r} \cos(\omega)x_k + \tilde{r} \sin(\omega)y_k] \right) \quad (7-21)\]

and

\[I_k(\tilde{r}, \omega) = \frac{1}{2\pi \hbar} \int_0^{2\pi} \int_{R^{(1)}_k(\theta)}^{R^{(2)}_k(\theta)} \exp \left( \frac{i}{\hbar} r(1 - \tilde{r} \cos(\theta - \omega)) \right) r dr d\theta. \quad (7-22)\]

With the above set-up in place, we have the following theorem namely,

**Theorem 7.1** (Circle Theorem). *If \(\tilde{r} \neq 1\), then,

\[\lim_{\hbar \to 0} F^\epsilon_h(\tilde{r}, \omega) = 0, \quad (7-23)\]

for any \(0 < \epsilon < \frac{1}{2}\).*

**7.2.1 Brief Exposition of the Theorem**

Before we furnish a rigorous proof for the aforementioned theorem, let us try to give simpler, intuitive picture of why the statement is true. Observe that the first exponential \(\exp \left( \frac{iS(x, y)}{\hbar} \right)\) in Equation 7–12 is a varying complex "sinusoid" and the second exponential \(\exp \left( \frac{-i(ux + vy)}{\hbar} \right)\) in Equation 7–12 is a fixed complex sinusoid at frequencies \(\frac{u}{\hbar}\) and \(\frac{v}{\hbar}\) respectively. When we multiply these two complex exponentials, at low values of \(\hbar\), the two sinusoids are usually not "in sync" and cancellations occur in
the integral. Exceptions to the cancellation happen at locations where $\nabla S = (S_x, S_y) = (u, v)$, as around these locations, the two sinusoids are in perfect sync. Since $\|\nabla S\| = 1$ for distance transforms, strong resonance occurs only when $u^2 + v^2 = 1$ ($\tilde{r} = 1$).

When $\tilde{r} \neq 1$, the two sinusoids tend to cancel each other out as $h \to 0$, resulting in $F_h^i$ becoming zero at those locations.

### 7.2.2 Formal Proof

Having given the intuitive picture of why the Theorem 7.1 holds good, we shall now provide the formal proof.

**Proof.** As each $C_k$ is bounded, it suffices to show that if $\tilde{r} \neq 1$, then $\lim_{h \to 0} I_k(\tilde{r}, \omega) = 0$ for all $I_k$.

Consider

$$ I = \frac{1}{2\pi \hbar} \int_0^{2\pi} \int_{R(1)(\theta)}^{R(2)(\theta)} \exp \left( \frac{i}{\hbar} r (1 - \tilde{r} \cos(\theta - \omega)) \right) r dr d\theta, \quad (7-24) $$

where $R(1)(\theta) = \epsilon R(\theta)$ and $R(2)(\theta) = (1 - \epsilon) R(\theta)$. Let the region $[0, 2\pi] \times [R(1)(\theta), R(2)(\theta)]$ be denoted by $D^\epsilon$. $R(\theta)$ is defined in such a way that the boundary of $D^\epsilon$ consists of a finite sequence of straight line segments as in the case of each $D_k^\epsilon$. Notice that $D^\epsilon$ doesn’t contain the origin $(0, 0)$.

Let $p(r, \theta) = r (1 - \tilde{r} \cos(\theta - \omega))$ denote the phase term of $I$ in Equation 7–24 for a given $\tilde{r}$ and $\omega$. The partial gradients of $p(r, \theta)$ are given by

$$ \frac{\partial p}{\partial r} = 1 - \tilde{r} \cos(\theta - \omega) \quad \frac{\partial p}{\partial \theta} = r \tilde{r} \sin(\theta - \omega). \quad (7-25) $$

Since $D$ is bounded away from the origin $(0, 0)$ $\nabla p$ is well-defined and bounded and it equals zero only when $\tilde{r} = 1$ and $\theta = \omega$. Since $\tilde{r} \neq 1$ by assumption, no stationary points exist ($\nabla p \neq 0$) and hence we can expect $I \to 0$ as $h \to 0$ [13, 25, 48]. We show the result more explicitly below.

Define a vector field $u(r, \theta) = \frac{\nabla p}{\|\nabla p\|} r$. Then it is easy to see that

$$ \nabla \cdot \left( u(r, \theta) \exp \left( \frac{ip(r, \theta)}{\hbar} \right) \right) = (\nabla u(r, \theta)) \exp \left( \frac{ip(r, \theta)}{\hbar} \right) + \frac{i}{\hbar} \exp \left( \frac{ip(r, \theta)}{\hbar} \right) r \quad (7-26) $$
where the gradient operator \( \nabla = \left[ \frac{\partial}{\partial r}, \frac{\partial}{\partial \theta} \right] \). Using the relation from Equation 7–26 in Equation 7–24, we get

\[
I = I^{(1)} - I^{(2)} \tag{7–27}
\]

where

\[
I^{(1)} = \frac{1}{2\pi il} \int_{\mathcal{D}^c} \nabla \cdot \left( \mathbf{u}(r, \theta) \exp \left( \frac{ip(r, \theta)}{\hbar} \right) \right) dr d\theta
\]

\[
I^{(2)} = \frac{1}{2\pi il} \int_{\mathcal{D}^c} \left( \nabla \mathbf{u}(r, \theta) \right) \exp \left( \frac{ip(r, \theta)}{\hbar} \right) dr d\theta. \tag{7–28}
\]

Consider the integral \( I^{(1)} \). From the divergence theorem we have

\[
I^{(1)} = \frac{1}{2\pi il} \int_{\Gamma} \left( \mathbf{u}^T \mathbf{n} \right) \exp \left( \frac{ip(r, \theta)}{\hbar} \right) ds \tag{7–29}
\]

where \( \Gamma \) is the positively oriented boundary of \( \mathcal{D}^c \), \( s \) is the arc length of \( \Gamma \) and \( \mathbf{n} \) is the unit outward normal of \( \Gamma \). The boundary \( \Gamma \) consists of two disjoint regions one along \( r(\theta) = R^{(1)}(\theta) \) and another along \( r(\theta) = R^{(2)}(\theta) \). If the level curves of \( p(r, \theta) \) is tangential to \( \Gamma \) only at a discrete set of locations giving rise to stationary points of the second kind \([29, 47, 48]\), in other words if values of \( p \) along the boundary \( \Gamma \) is not constant over any contiguous interval of \( \theta \), then using one dimensional stationary phase approximations \([31, 32]\) \( I^{(1)} \) can be shown to be \( O(\sqrt{\hbar}) \) and hence converges to zero as \( \hbar \to 0 \). Since the boundary of \( \mathcal{D}^c \) is made of straight line segments (specifically not arc-like), we can show that the level curves of \( p(r, \theta) \) cannot overlap with \( \Gamma \) for a non-zero finite interval. The subsequent paragraph takes care of this technical issue and the reader may decide to omit it upon first reading.

The level curves of \( p(r, \theta) \) are given by \( R(\theta)(1 - \tilde{r} \cos(\theta - \omega)) = c \), where \( c \neq 0 \) is some constant. Recall that each of the two disjoint regions of \( \Gamma \) is made of a finite sequence of line segments. For the level curves of \( p(r, \theta) \) to coincide with \( \Gamma \) over a non-zero finite interval, \( y(\theta) = \frac{c \sin(\theta)}{1 - \tilde{r} \cos(\theta - \omega)} \) and \( x(\theta) = \frac{c \cos(\theta)}{1 - \tilde{r} \cos(\theta - \omega)} \) should satisfy the line equation \( y = mx + b \) for some slope \( m \) and slope-intercept \( b \), when \( \theta \) varies over some
contiguous interval $\theta \in [\theta_1, \theta_2]$. Plugging in the value of $y$ and $x$ to the line equation and expanding $\cos(\theta - \omega)$ we get

$$c \sin \theta = mc \cos(\theta) + b - b \tilde{r} [\cos(\theta) \cos(\omega) + \sin(\theta) \sin(\omega)]. \quad (7-30)$$

Combining terms we get

$$\sin(\theta) [c + b \tilde{r} \sin(\omega)] - \cos(\theta) [mc - b \tilde{r} \cos(\omega)] = b. \quad (7-31)$$

By defining $\lambda_1 = c + b \tilde{r} \sin(\omega)$ and $\lambda_2 = -(mc - b \tilde{r} \cos(\omega))$ we see that $\sin(\theta)$ and $\cos(\theta)$ needs to satisfy the linear relation

$$\lambda_1 \sin(\theta) + \lambda_2 \cos(\theta) = b \quad (7-32)$$

for $\theta \in [\theta_1, \theta_2]$ in order for the level curves of $p(r, \theta)$ to overlap with the piece-wise linear boundary $\Gamma$. As Equation 7–32 cannot be true for a finite interval of $\theta$, $I^{(1)} = O(\sqrt{h})$ as $h \to 0$ and hence converges to zero in the limit.

Now $I^{(2)}$ has the similar form as the original $I$ in Equation 7–24 with $r$ replaced by $g_1 = (\nabla \cdot \mathbf{u})$. By letting $\mathbf{u}_1(r, \theta) = \frac{\nabla p}{\|\nabla p\|^2} g_1$, from Equation 7–26 and the divergence theorem we get

$$I^{(2)} = -\frac{h}{2\pi \Gamma} \int_{r} (\mathbf{u}_1 \cdot \mathbf{n}) \exp \left( \frac{ip(r, \theta)}{h} \right) ds + \frac{h}{2\pi \Gamma} \iint_{D^*} (\nabla \cdot \mathbf{u}_1(r, \theta)) \exp \left( \frac{ip(r, \theta)}{h} \right) drd\theta. \quad (7-33)$$

As $I^{(2)} = O(h)$, it converges to zero as $h \to 0$. Applying the obtained results to Equation 7–27 we see that $I$ (and hence $l_k$) $\to 0$ as $h \to 0$ which completes the proof.

Since the Theorem 7.1 is true for any $0 < \epsilon < \frac{1}{2}$, it also holds good as $\epsilon \to 0$. Hence as a corollary we have the following result namely,
Corollary 1. If $\bar{r} \neq 1$, then
\[
\lim_{\epsilon \to 0} \lim_{h \to 0} F^\epsilon_h(\bar{r}, \omega) = 0. \tag{7–34}
\]

7.3 Spatial Frequencies as Gradient Histogram Bins

We now show that the square magnitude of the Fourier transform of the CWR ($\phi$) when polled close to the unit circle ($\bar{r} = 1$) is approximately equal to the density function of the distance transform gradients $P$ with the approximation tightening up as $h \to 0$.

The squared magnitude of the Fourier transform also called its power spectrum [7] is given by
\[
P^\epsilon_h(\bar{r}, \omega) \equiv |F^\epsilon_h(\bar{r}, \omega)|^2 = F^\epsilon_h(\bar{r}, \omega)\overline{F^\epsilon_h(\bar{r}, \omega)}. \tag{7–35}
\]

By definition $P^\epsilon_h(\bar{r}, \omega) \geq 0$. From Lemma 5, we have
\[
\int_0^{2\pi} \int_0^{\infty} P^\epsilon_h(\bar{r}, \omega) \bar{r} d\bar{r} d\omega = 1 \tag{7–36}
\]
independent of $h$. Hence $P^\epsilon_h(\bar{r}, \omega)\bar{r}$ can be treated as a density function for all values of $h$. In the parlance of quantum mechanics, this quantity $P^\epsilon_h$ carries an interpretation of being the quantum momentum density of the wave function $\phi$ (refer Section 6.2).

The correspondence principle described under Section 6.1 dictates that the quantum density $P^\epsilon_h$ must approach its classical counterpart $P$ in the limit as $h \to 0$. We earlier observed that the gradient density function of the unit vector distance transform gradients is one-dimensional and defined only over the space of orientations. For $P^\epsilon_h(\bar{r}, \omega)\bar{r}$ to behave as an orientation density function, it needs to be integrated along the radial direction $\bar{r}$. Since Theorem 7.1 states that the Fourier transform values are concentrated only on the unit circle $\bar{r} = 1$ and converges to zero elsewhere as $h \to 0$, it should be sufficient if the integration for $\bar{r}$ is done over a region very close to one. The following theorem confirms our current observations.
Theorem 7.2 (Quantum meets classical). For any given \(0 < \epsilon < \frac{1}{2}, 0 < \delta < 1\), \(\omega_0 \in [0, 2\pi)\) and \(0 < \Delta < 2\pi\),

\[
\lim_{\hbar \to 0} \int_{\omega_0}^{\omega_0 + \Delta} \int_{1-\delta}^{1+\delta} P_{\hbar}^2(\tilde{r}, \omega) \tilde{r} d\tilde{r} d\omega = \int_{\omega_0}^{\omega_0 + \Delta} P(\omega) d\omega. \tag{7–37}
\]

7.3.1 Brief Exposition of the Theorem

Before we proceed with the formal analysis of the proof, we once again try to give a intuitive reasoning of why the theorem statement is true. The Fourier transform of the CWR defined in Equation 7–12 involves two spatial integrals (over \(x\) and \(y\)) which are converted into polar coordinate domain integrals. The squared magnitude of the Fourier transform (power spectrum), \(P_{\hbar}(\tilde{r}, \omega)\), involves multiplying the Fourier transform with its complex conjugate. The complex conjugate is yet another 2D integral which we will perform in the polar coordinate domain. As the gradient density function is one-dimensional and defined over the space of orientations, we integrate the power spectrum along the radial direction close to the unit circle \(\tilde{r} = 1\) (as \(\delta \to 0\)). This is a fifth integral. When we poll the power spectrum \(P_{\hbar}(\tilde{r}, \omega)\) close to \(\tilde{r} = 1\), the two sinusoids namely \(\exp \left( \frac{iS(x,y)}{\hbar} \right)\) and \(\exp \left( -i\left(\frac{ux + vy}{\hbar} \right) \right)\) in Equation 7–12 are in resonance only when there is a perfect match between the orientation of each ray of the distance transform \(S(x,y)\) and the angle of the 2D spatial frequency \((\omega = \arctan \left( \frac{v}{u} \right))\). All the grid locations \((x, y)\) having the same gradient orientation

\[
\arctan \left( \frac{S_y}{S_x} \right) = \arctan \left( \frac{v}{u} \right)
\]

(7–38)

casts a vote only at its corresponding spatial frequency "histogram" bin \(\omega\). Since the histogram bin is generally indexed by multiple grid locations, it leads to cross phase factors. Integrating the power spectrum over a small range on the orientation helps in cancelling out these phase factors giving us the desired result when we take the limit as \(\hbar \to 0\). This integral and limit cannot be exchanged because the phase factors will not otherwise cancel. The proof mainly deals with managing these six integrals.
7.3.2 Formal Proof

We now provide the formal proof of our Theorem 7.2.

Proof. Firstly observe that

\[
F_h^c(\bar{r}, \omega) = \sum_{k=1}^{K} \frac{C_k}{2\pi h^k} \int_0^{2\pi} \int_{R_k^{(1)}}^{R_k^{(0)}} \exp \left( \frac{-ir'r}{h} [1 - \bar{r} \cos(\theta' - \omega)] \right) r' dr' d\theta'.
\]  

(7–39)

Define

\[
l(\omega) \equiv \int_{1-\delta}^{1+\delta} P_h^c(\bar{r}, \omega) \bar{r} d\bar{r}.
\]  

(7–40)

As \( h \to 0 \), \( l(\omega) \) will approach the density function of the gradients of \( S(x, y) \). Note that the integral in Equation 7–40 is over the interval \([1 - \delta, 1 + \delta]\) where \( \delta > 0 \) can be made arbitrarily small (as \( h \to 0 \)) due to Theorem 7.1. Since \( P_h^c(\bar{r}, \omega) \) equals \( F_h^c(\bar{r}, \omega) \), we have

\[
l(\omega) = \sum_{j=1}^{K} \sum_{k=1}^{K} \frac{1}{(2\pi h^k)^2} G_{jk}(\omega),
\]  

(7–41)

where

\[
G_{jk}(\omega) = \int_{1-\delta}^{1+\delta} \int_0^{2\pi} \int_{R_k^{(1)}}^{R_k^{(0)}} \int_0^{2\pi} \int_{R_k^{(1)}}^{R_k^{(0)}} \exp \left( \frac{i}{h} b_{jk} \right) f_1 dr d\theta' dr' d\theta' d\bar{r}.
\]  

(7–42)

Here,

\[
b_{jk}(r, \theta, r', \theta', \bar{r}) = r [1 - \bar{r} \cos(\theta - \omega)] - r' [1 - \bar{r} \cos(\theta' - \omega)]
\]

\[
- \bar{r} [\cos(\omega)(x_j - x_k) + \sin(\omega)(y_j - y_k)],
\]  

(7–43)

and

\[
f_1(r, r', \bar{r}) = rr' \bar{r}.
\]  

(7–44)

Notice that the phase term of the quantity \( C_j \overline{C_k} \), namely

\[
- \bar{r} [\cos(\omega)(x_j - x_k) + \sin(\omega)(y_j - y_k)]
\]  

(7–45)

is absorbed in \( b_{jk} \). Since we are interested only in the limit as \( h \to 0 \), essential contribution to \( G_{jk}(\omega) \) comes only from the stationary (critical) point(s) of \( b_{jk} \) [47].
The partial derivatives of $b_{jk}(r, \theta, r', \theta', \bar{r})$ are given by

\[
\frac{\partial b_{jk}}{\partial r} = 1 - \bar{r} \cos(\theta - \omega), \quad \frac{\partial b_{jk}}{\partial \theta} = r \bar{r} \sin(\theta - \omega), \\
\frac{\partial b_{jk}}{\partial r'} = -1 + \bar{r} \cos(\theta' - \omega), \quad \frac{\partial b_{jk}}{\partial \theta'} = -r' \bar{r} \sin(\theta' - \omega), \\
\frac{\partial b_{jk}}{\partial \bar{r}} = -r \cos(\theta - \omega) + r' \cos(\theta' - \omega) - [\cos(\omega)(x_j - x_k) + \sin(\omega)(y_j - y_k)].
\]

(7–46)

As $r$, $r'$ and $\bar{r} > 0$, it is easy to see that for $\nabla b_{jk} = 0$ (stationary), we must have

\[
\bar{r} = 1, \quad \theta = \theta' = \omega, \quad r = r' - [\cos(\omega)(x_j - x_k) + \sin(\omega)(y_j - y_k)].
\]

(7–47)

Let $t_0$ denote the stationary point. The Hessian matrix $W$ of $b_{jk}$ at $t_0$ is given by

\[
W(r, \theta, r', \theta', \bar{r})|_{t_0} = \begin{bmatrix}
0 & 0 & 0 & 0 & -1 \\
0 & r_{t_0} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & -r' & 0 \\
-1 & 0 & 1 & 0 & 0
\end{bmatrix}
\]

where $r_{t_0} = r' - [\cos(\omega)(x_j - x_k) + \sin(\omega)(y_j - y_k)]$. Unfortunately, the determinant of $W$ at the stationary point $t_0$ equals 0 as the first and third rows—corresponding to $r$ and $r'$ respectively—are scalar multiples of each other. Also note that the value of $r'$ is not determined at the stationary point. This impedes us from directly applying the 5D stationary phase approximation [47]. Hence we propose to solve for $I(\omega)$ in Equation 7–40 by manual symmetry breaking, where we fix the conjugate variables $r'$ and $\theta'$ and perform the integration only with respect to the other three variables namely $r$, $\theta$ and $\bar{r}$.

To this end, let

\[
l(\omega) = \sum_{j=1}^{K} \sum_{k=1}^{K} \frac{1}{(2\pi \hbar)^2} \int_{0}^{2\pi} \int_{R_{\hbar}^{(2)}(\theta')} \exp \left( \frac{-ir'}{\hbar} \right) g_{jk}(r', \theta')r'dr'd\theta',
\]

(7–48)
where

\[
  g_{jk}(r', \theta') = \int_{1-\delta}^{1+\delta} \int_{0}^{2\pi} \int_{R_j^{(2)}(\theta)}^{R_j^{(1)}(\theta)} \exp \left( i \gamma_{jk}(r, \theta, \bar{r}) \right) f_2(r, \theta, \bar{r}) drd\theta d\bar{r}.
\]  

(7–49)

Here,

\[
  \gamma_{jk}(r, \theta, \bar{r}) = r \left[ 1 - \bar{r} \cos(\theta - \omega) \right] + r' \bar{r} \cos(\theta' - \omega) - \bar{r} \left[ \cos(\omega)(x_j - x_k) + \sin(\omega)(y_j - y_k) \right]
\]

(7–50)

and

\[
  f_2(r, \theta, \bar{r}) = r \bar{r}.
\]

(7–51)

In the definition for \( \gamma_{jk}(r, \theta, \bar{r}) \) in Equation 7–50, \( \omega, r' \) and \( \theta' \) are held fixed and for \( g_{jk}(r', \theta') \) in Equation 7–49, \( \omega \) is held constant. The phase term of the quantity \( C_j \bar{C}_k \) (Equation 7–45) is absorbed in \( \gamma_{jk} \) and pursuant to Fubini’s theorem, the integration with respect to \( \bar{r} \) is considered before the integration for \( r' \) and \( \theta' \).

As stated before, essential contribution to \( g_{jk}(r', \theta') \) comes only from the stationary points of \( \gamma_{jk} \) as \( h \to 0 \) [47]. The partial derivatives of \( \gamma_{jk}(r, \theta, \bar{r}) \) are given by

\[
  \frac{\partial \gamma_{jk}}{\partial r} = 1 - \bar{r} \cos(\theta - \omega), \quad \frac{\partial \gamma_{jk}}{\partial \theta} = r \bar{r} \sin(\theta - \omega)
\]

\[
  \frac{\partial \gamma_{jk}}{\partial \bar{r}} = -r \cos(\theta - \omega) + r' \cos(\theta' - \omega) - \left[ \cos(\omega)(x_j - x_k) + \sin(\omega)(y_j - y_k) \right].
\]

(7–52)

As both \( r \) and \( \bar{r} \) \( > 0 \), for \( \nabla \gamma_{jk} = 0 \) (stationary), we must have

\[
  \bar{r} = 1, \quad \theta = \omega, \quad \text{and} \quad r = r' \cos(\theta' - \omega) - \left[ \cos(\omega)(x_j - x_k) + \sin(\omega)(y_j - y_k) \right].
\]

(7–53)

Let \( p_0 \) denote the stationary point. Then

\[
  \gamma_{jk}(p_0) = r' \cos(\theta' - \omega) - \left[ \cos(\omega)(x_j - x_k) + \sin(\omega)(y_j - y_k) \right] = r_{p_0},
\]

\[
  f_2(p_0) = r_{p_0} = \gamma_{jk}(p_0)
\]

(7–54)
and the Hessian matrix $H$ of $\gamma_{jk}$ at $p_0$ is given by

$$H(r, \theta, \tilde{r})|_{p_0} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & \gamma_{jk}(p_0) & 0 \\ -1 & 0 & 0 \end{bmatrix}$$

The determinant of $H$ equals $-\gamma_{jk}(p_0)$. Since $r$ (specifically $r_{p_0}$) $> 0$, we see that the determinant of $H$ is strictly negative and its signature—difference between the number of positive and negative eigenvalues—is one. Then from higher dimensional stationary phase approximation [47], we have

$$g_{jk}(r', \theta') = (2\pi\hbar)^{\frac{3}{2}}\sqrt{\gamma_{jk}(p_0)} \exp \left( \frac{i\gamma_{jk}(p_0)}{\hbar} + \frac{i\pi}{4} \right) + \epsilon_1(r', \theta', \omega, \hbar) \quad (7-55)$$

as $\hbar \to 0$, where $\epsilon_1(r', \theta', \omega, \hbar)$ includes the contributions from the boundary in Equation 7–49. Here we have assumed that the stationary point $p_0$ doesn’t occur on the boundary but lies to its interior, i.e, $R_j^{(1)}(\omega) < r_{p_0} < R_j^{(2)}(\omega)$ as the measure on the set of $\{\omega, \theta', r'\}$ for which $r_{p_0}$ ( or $p_0$) may occur on the boundary is zero. Let $\Gamma$ denote the boundary in Equation 7–49. If there doesn’t exist a 2D patch on $\Gamma$ on which $\gamma_{jk}$ is constant, then we can conclude that $\epsilon_1(r', \theta', \omega, \hbar)$—which contributions from the boundary $\Gamma$ involving the stationary points of second kind where the level curves of $\gamma_{jk}$ are tangential to $\Gamma$—should at least be $O(\hbar^2)$ as $\hbar \to 0$ [13, 25, 47]. Furthermore,

$$\epsilon_1(r', \theta', \omega, \hbar) = \hbar^\kappa \xi(r', \theta', \omega) \quad (7-56)$$

where $\kappa \geq 2$ and $\xi$ is some bounded continuous function of $r'$ and $\theta'$ and $\omega$. Since the boundary $\Gamma$ is made of straight line segments, we can show that this is indeed the case. The subsequent paragraph takes care of this technical issue and may be omitted upon first reading.

The boundary $\Gamma$ in Equation 7–49 is the union of two disconnected surfaces $\Gamma_1 = A_1 \times [1 - \delta, 1 + \delta]$ and $\Gamma_2 = A_2 \times [1 - \delta, 1 + \delta]$ where $A_1$ is the boundary along $r(\theta) = R_j^{(1)}(\theta)$ and $A_2$ is the boundary along $r(\theta) = R_j^{(2)}(\theta)$. Note that both $A_1$ and $A_2$
are composed of a finite sequence of straight line segments. Consider the surface $\Gamma_1$.

The value of $\gamma_{jk}$ on the surface $\Gamma_1$ at a given $\theta$ and $\tilde{r}$ equals

$$\gamma_{jk}^{\Gamma_1}(\theta, \tilde{r}) = R_j^{(1)}(\theta)[1 - \tilde{r}\cos(\theta - \omega)] + \lambda\tilde{r}, \quad(7-57)$$

where

$$\lambda = r' \cos(\theta' - \omega) - [\cos(\omega)(x_j - x_k) + \sin(\omega)(y_j - y_k)]. \quad(7-58)$$

Following the lines of Theorem 7.1, we observe that for a given $\tilde{r}$, $\gamma_{jk}^{\Gamma_1}(\theta, \tilde{r})$ cannot be constant for a contiguous interval of $\theta$ as the Equation 7–32 cannot be satisfied for any finite interval. By similar argument there can exist at most only a finite discrete set of $\theta$ for which $R_j^{(1)}(\theta) \cos(\theta - \omega) = \lambda$. Let $\mathcal{Z}$ denote this finite set. Then for a given $\theta \notin \mathcal{Z}$, $\gamma_{jk}^{\Gamma_1}$ varies linearly in $\tilde{r}$ and specifically, its derivative with respect to $\tilde{r}$ doesn't vanish.

From the above observations we can conclude that there doesn’t exist a 2D patch on $\Gamma_1$ on which $\gamma_{jk}^{\Gamma_1}$ is constant. Similar conclusion can be obtained even for the surface $\Gamma_2$. Hence $\gamma_{jk}$ cannot be constant on the boundary $\Gamma$ over a 2D region having a finite non-zero measure.

Now, plugging the value of $g(r', \theta')$ in Equation 7–48 we get

$$I(\omega) = \sum_{j=1}^{K} \sum_{k=1}^{K} \left\{ \frac{\eta_{jk}(\omega)}{L^2} \left[ I_{jk}^{(1)}(\omega) + I_{jk}^{(2)}(\omega) \right] \right\} \quad(7-59)$$

where,

$$I_{jk}^{(1)}(\omega) = \frac{1}{\sqrt{2\pi}h} \int_{0}^{2\pi} \int_{R_k^{(1)}(\theta')} \exp \left( \frac{ip(r', \theta', \omega)}{h} \right) q(r', \theta', \omega) dr'd\theta', \quad(7-60)$$

$$I_{jk}^{(2)}(\omega) = \int_{0}^{2\pi} \int_{R_k^{(1)}(\theta')} \exp \left( -\frac{ir'}{h} \right) r'\epsilon_2(r', \theta', \omega, h) dr'd\theta',$$

$$\eta_{jk}(\omega) = \exp \left( -\frac{i\alpha_{jk}(\omega)}{h} + \frac{i\pi}{4} \right),$$

$$\alpha_{jk}(\omega) = \cos(\omega)(x_j - x_k) + \sin(\omega)(y_j - y_k),$$

$$\epsilon_2(r', \theta', \omega, h) = \frac{\epsilon_1(r', \theta', \omega, h)}{(2\pi h\hbar)^2} = \frac{1}{(2\pi h)^2} h^{\kappa-2} \xi(r', \theta', \omega).$$
The functions $p(r', \theta', \omega)$ and $q(r', \theta', \omega)$ are given by
\[
p(r', \theta', \omega) = -r'[1 - \cos(\theta' - \omega)] \text{ and } q(r', \theta', \omega) = r' \sqrt{r' \cos(\theta' - \omega) - \alpha_j(\omega)}. \tag{7-61}
\]

Since $\kappa \geq 2$, we can conclude that for small values of $\epsilon_\omega(r', \theta', \omega, \hbar)$ can be bounded by $\xi(r', \theta', \omega)$ and pursuant to the Riemann-Lesbegue lemma, $\lim_{\hbar \to 0} I_{jk}^{(2)} = 0$. Moreover from the Lesbegue dominated convergence theorem it follows that
\[
\lim_{h \to 0} \int_{\omega_0}^{\omega_0+\Delta} \sum_{j=1}^{K} \sum_{k=1}^{K} I_{jk}^{(2)}(\omega) = \sum_{j=1}^{K} \sum_{k=1}^{K} \int_{0}^{2\pi} \lim_{h \to 0} I_{jk}^{(2)}(\omega) = 0. \tag{7-62}
\]

Using the above result in Equation \ref{eq:7-59} we get,
\[
\lim_{h \to 0} \int_{\omega_0}^{\omega_0+\Delta} I(\omega) d\omega = \sum_{j=1}^{K} \sum_{k=1}^{K} \lim_{h \to 0} \int_{\omega_0}^{\omega_0+\Delta} \frac{\eta_{jk}}{L^e} I_{jk}^{(1)}(\omega) d\omega, \tag{7-63}
\]
which leaves us to show that
\[
\sum_{j=1}^{K} \sum_{k=1}^{K} \lim_{h \to 0} \int_{\omega_0}^{\omega_0+\Delta} \frac{\eta_{jk}(\omega)}{L^e} I_{jk}^{(1)}(\omega) d\omega = \int_{\omega_0}^{\omega_0+\Delta} P(\omega) d\omega. \tag{7-64}
\]

Consider the integral $I_{jk}^{(1)}(\omega)$. Fix a $\beta > 0$. Dividing the integral range $[0, 2\pi)$ for $\theta'$ into three disjoint regions namely $[0, \omega - \beta)$, $[\omega - \beta, \omega + \beta]$ and $(\omega + \beta, 2\pi)$, we get
\[
I_{jk}^{(1)}(\omega) = I_{jk}^{(1)}(\beta, \omega) + I_{jk}^{(2)}(\beta, \omega) + I_{jk}^{(3)}(\beta, \omega), \tag{7-65}
\]
where,
\[
I_{jk}^{(1)}(\beta, \omega) = \frac{1}{\sqrt{2\pi \hbar}} \int_{-\beta}^{\omega+\beta} \int_{R_{k}^{(2)}(\theta')} \exp \left( \frac{ip(r', \theta', \omega)}{\hbar} \right) q(r', \theta', \omega) dr' d\theta',
\]
\[
I_{jk}^{(2)}(\beta, \omega) = \frac{1}{\sqrt{2\pi \hbar}} \int_{-\beta}^{\omega+\beta} \int_{R_{k}^{(2)}(\theta')} \exp \left( \frac{ip(r', \theta', \omega)}{\hbar} \right) q(r', \theta', \omega) dr' d\theta',
\]
\[
I_{jk}^{(3)}(\beta, \omega) = \frac{1}{\sqrt{2\pi \hbar}} \int_{-\beta}^{\omega+\beta} \int_{R_{k}^{(2)}(\theta')} \exp \left( \frac{ip(r', \theta', \omega)}{\hbar} \right) q(r', \theta', \omega) dr' d\theta'. \tag{7-66}
\]
Since it is true for any $\beta > 0$, we can consider the case as $\beta \to 0$. Fix a $\beta$ close enough to zero and consider the above integrals as $h \to 0$. As essential contributions to the above integrals comes only from the stationary points of $\rho(r', \theta', \omega)$ [13, 25, 48] (with $\omega$ held fixed), we first determine its critical (stationary) point(s). The gradients of $\rho(r', \theta', \omega)$ at a fixed $\omega$ are given by

$$\frac{\partial \rho}{\partial r'} = -1 + \cos(\theta' - \omega) \quad \frac{\partial \rho}{\partial \theta'} = -r' \sin(\theta' - \omega). \quad (7-67)$$

For $\nabla \rho = 0$, we must have $\theta' = \omega$. By construction the integrals $J^{(2)}_{jk}(\beta, \omega)$ and $J^{(3)}_{jk}(\beta, \omega)$ do not include the stationary point $\theta' = \omega$ and hence $\nabla \rho \neq 0$ in these integrals. Following the lines of Theorem 7.1, by defining the vector field $u = \frac{\nabla \rho}{\|\nabla \rho\|}$ and then applying the divergence theorem, both $J^{(2)}_{jk}(\beta, \omega)$ and $J^{(3)}_{jk}(\beta, \omega)$ can be shown to be $h^{\kappa_2} \zeta^{(2)}(\beta, \omega)$ and $h^{\kappa_3} \zeta^{(3)}(\beta, \omega)$ respectively where both $\kappa_2$ and $\kappa_3 \geq 0.5$ and $\zeta^{(2)}$ and $\zeta^{(3)}$ are some continuous bounded function of $\beta$ and $\omega$. Hence we can conclude that

$$\left| \lim_{h \to 0} \int_0^{2\pi} \eta_{jk} \frac{\eta_{jk}}{L^k} J^{(2)}_{jk}(\beta, \omega) d\omega \right| \leq \lim_{h \to 0} \frac{h^{\kappa_2}}{L^k} \int_0^{2\pi} |\zeta^{(2)}(\beta, \omega)| d\omega = 0 \quad (7-68)$$

as $|\eta_{jk} = 1|$ and similarly for $J^{(3)}_{jk}(\beta, \omega)$ for any fixed $\beta > 0$. It follows that the result also holds as $\beta \to 0$ provided the limit for $\beta$ is consider after the limit for $h$, i.e,

$$\lim_{\beta \to 0} \lim_{h \to 0} \int_{\omega_0}^{\omega_0 + \Delta} \frac{\eta_{jk}}{L^k} J^{(2)}_{jk}(\beta, \omega) d\omega = 0$$

$$\lim_{\beta \to 0} \lim_{h \to 0} \int_{\omega_0}^{\omega_0 + \Delta} \frac{\eta_{jk}}{L^k} J^{(3)}_{jk}(\beta, \omega) d\omega = 0. \quad (7-69)$$

Hence $J^{(1)}_{jk}(\omega)$ in Equation 7–65 can be approximated by $J^{(1)}_{jk}(\beta, \omega)$ as $\beta \to 0$ and as $h \to 0$. Using this result in Equation 7–64 leaves us to prove that

$$\sum_{j=1}^{K} \sum_{k=1}^{K} \lim_{\beta \to 0} \lim_{h \to 0} \int_{\omega_0}^{\omega_0 + \Delta} \frac{\eta_{jk}(\omega)}{L^k} J^{(1)}_{jk}(\beta, \omega) d\omega = \int_{\omega_0}^{\omega_0 + \Delta} P(\omega) d\omega. \quad (7-70)$$

We now evaluate $J^{(1)}_{jk}(\beta, \omega)$ by interchanging the order of integration between $r'$ and $\theta'$ which requires us to rewrite $\theta'$ as a function of $r'$. Recall that for each data
point \( Y_k \), the boundaries of the region \( D_k \) along \( r(\theta') = R_k^{(1)}(\theta') \) and \( r(\theta') = R_k^{(2)}(\theta') \) respectively is comprised of a finite sequence of straight line segments. In order to evaluate \( J_{jk}^{(1)}(\beta, \omega) \) we need to consider these boundaries only within the precincts of the angles \([\omega - \beta, \omega + \beta]\) on each \( D_k \). But for sufficiently small \( \beta \), we observe that for every \( \omega \in [0, 2\pi) \), when we consider these boundaries (along \( R_k^{(1)}(\theta') \) and \( R_k^{(2)}(\theta') \) respectively) within the angles \([\omega - \beta, \omega + \beta]\), they will be comprised of at most two line segments (see Figure 7-3).

![Figure 7-3. Boundary considered within the angles \([\omega - \beta, \omega + \beta]\) is comprised of at most two line segments \( L_1 \) and \( L_2 \).](image)

Over each line segment, \( r'(\theta') \) is either strictly monotonic (strictly increases or strictly decreases) or has exactly one critical point (strictly decreases, attains a minimum and then strictly increases) as shown in Figure 7-4.

Hence it follows that for sufficiently small \( \beta \), \( \theta' \) rewritten as a function of \( r' \) may be composed of at most three disconnected regions (refer Figure 7-5).

Let \( \mathcal{B}(r') \subseteq [\omega - \beta, \omega + \beta] \) denote the integral region for \( \theta'(r') \). Treating \( \theta' \) as a function of \( r' \) and applying Fubini’s theorem, the integral \( J_{jk}^{(1)}(\beta, \omega) \) can be rewritten as

\[
J_{jk}^{(1)}(\beta, \omega) = \int_{r_k^{(1)}(\beta, \omega)}^{r_k^{(2)}(\beta, \omega)} G(r', \omega) dr', \tag{7–71}
\]
Figure 7-4. Plot of radial length \((r)\) vs angle \((\theta)\).

Figure 7-5. Three disconnected regions for the angle \((\theta)\).

where

\[
\begin{align*}
r_k^{(1)}(\beta, \omega) &= \inf \{ R_k^{(1)}(\theta') \}, \\
r_k^{(2)}(\beta, \omega) &= \sup \{ R_k^{(2)}(\theta') \}
\end{align*}
\]  

(7–72)

when \(\theta' \in [\omega - \beta, \omega + \beta]\) and

\[
G(r', \omega) = \frac{1}{\sqrt{2\pi \hbar}} \int_{\mathcal{S}(r')} \exp \left( \frac{ip(r', \theta', \omega)}{\hbar} \right) q(r', \theta', \omega) d\theta'.
\]  

(7–73)
Note that while evaluating the integral $G(r', \omega)$, $r'$ and $\omega$ are held fixed. As contributions to $G$ comes only from the stationary points of $p(r', \theta', \omega)$ (with $r'$ and $\omega$ held fixed) as $\hbar \to 0$, we evaluate $\frac{\partial p}{\partial \theta'} = -r' \sin(\theta' - \omega)$ and for it to vanish $\theta' = \omega$. Moreover

$$\frac{\partial^2 p}{\partial \theta^2} |_{\omega} = -r', \quad p(r', \omega, \omega) = 0$$

and

$$q(r', \omega, \omega) = r' \sqrt{r' - \alpha_{jk}(\omega)} \quad (7-74)$$

For the given $r'$, if $\omega \notin B(r')$, then no stationary points exists. Using integration by parts $G(r', \omega)$ can be shown to be $\epsilon_3(r', \omega, \hbar) = O(\sqrt{\hbar})$ which can be uniformly bounded by a function of $r'$ for small values of $\hbar$.

If $\omega \in B(r')$, then using one dimensional stationary phase approximations [31, 32] it can be shown that

$$G(r', \omega) = \exp \left( -\frac{i \pi}{4} \right) \sqrt{r'} \sqrt{r' - \alpha_{jk}(\omega)} + \epsilon_4(r', \omega, \hbar) \quad (7-75)$$

where $\epsilon_4(r', \omega, \hbar)$ can be uniformly bounded by a function of $r'$ for small values of $\hbar$ and converges to zero as $\hbar \to 0$. Here we have assumed that the stationary point $\theta' = \omega$ lies to the interior of $B(r')$ and not on the boundary as there can be at most finite (actually 2) values of $r'$ (with Lesbegue measure zero) for which $\theta' = \omega$ can lie in the boundary of $B(r')$. Plugging the value of $G(r', \omega)$ in Equation 7–71 we get

$$\int_{\omega_0}^{\omega_0 + \Delta} \frac{\eta_{jk}(\omega)}{L^\epsilon} f_{jk}^{(1)}(\beta, \omega) d\omega = \frac{1}{L^\epsilon} \int_0^{2\pi} \exp \left( -\frac{i \alpha_{jk}(\omega)}{\hbar} \right) \rho_{jk}(\beta, \omega) d\omega$$

$$+ \int_{\omega_0}^{\omega_0 + \Delta} \frac{\eta_{jk}(\omega)}{L^\epsilon} \left\{ \int_{r_k^{(1)}(\beta, \omega)}^{r_k^{(2)}(\beta, \omega)} \chi(r', \omega, \hbar) dr' \right\} d\omega, \quad (7-76)$$

where

$$\rho_{jk}(\beta, \omega) = \int_{r_k^{(1)}(\beta, \omega)}^{r_k^{(2)}(\beta, \omega)} \sqrt{r'} \sqrt{r' - \alpha_{jk}(\omega)} dr', \quad (7-77)$$

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\( r_k^-(\beta, \omega) \geq r_k^1(\beta, \omega) \) and \( r_k^+(\beta, \omega) \leq r_k^2(\beta, \omega) \) are the values of \( r' \) such that when \( r_k^-(\beta, \omega) < r' < r_k^+(\beta, \omega) \), the stationary point \( \theta' = \omega \) lies to the interior of \( B(r') \) and

\[
\chi(r', \omega, h) = \begin{cases} 
\epsilon_4(r', \omega, h); & r_k^-(\beta, \omega) < r' < r_k^+(\beta, \omega) \\
\epsilon_3(r', \omega, h); & r' < r_k^-(\beta, \omega) \text{ or } r_k^+(\beta, \omega) < r'.
\end{cases}
\]

Since \( |\eta_{jk}(\omega) = 1| \) and \( \chi(r', \omega, h) \) can be uniformly bounded by a function \( r' \) and \( \omega \) for small values of \( h \), by the Lebesgue dominated convergence theorem we have

\[
\lim_{h \to 0} \int_{\omega_0}^{\omega_0 + \Delta} \frac{\eta_{jk}(\omega)}{L\epsilon} \left\{ \int_{r_k^1(\beta, \omega)}^{r_k^2(\beta, \omega)} \chi(r', \omega, h) \, dr' \right\} \, d\omega = \int_{\omega_0}^{\omega_0 + \Delta} \frac{\eta_{jk}(\omega)}{L\epsilon} \left\{ \int_{r_k^1(\beta, \omega)}^{r_k^2(\beta, \omega)} \lim_{h \to 0} \chi(r', \omega, h) \, dr' \right\} \, d\omega = 0. \tag{7–78}
\]

This leaves us only with the first integral in Equation 7–76. Let \( \tau_{jk}(\beta) \) denote this integral, namely

\[
\tau_{jk}(\beta) = \frac{1}{L\epsilon} \int_{\omega_0}^{\omega_0 + \Delta} \exp \left( \frac{-j\alpha_{jk}}{\hbar} \right) \rho_{jk}(\beta, \omega) \, d\omega. \tag{7–79}
\]

We need to show that

\[
\sum_{j=1}^{K} \sum_{k=1}^{K} \lim_{\beta \to 0} \lim_{h \to 0} \tau_{jk}(\beta) = \int_{\omega_0}^{\omega_0 + \Delta} P(\omega) \, d\omega. \tag{7–80}
\]

We now consider two cases where \( j = k \) and \( j \neq k \).

case (i): If \( j \neq k \), then \( \alpha_{jk}(\omega) \) varies continuously with \( \omega \). Also notice that \( \rho_{jk}(\beta, \omega) \) is independent of \( h \) and a bounded function of \( \beta \) and \( \omega \). The stationary point(s) of \( \alpha_{jk} \)—denoted by \( \tilde{\omega} \)—satisfies

\[
\tan(\tilde{\omega}) = \frac{y_j - y_k}{x_j - x_k} \tag{7–81}
\]

and the second derivative of \( \alpha_{jk}(\omega) \) at its stationary point is given by

\[
\alpha_{jk}''(\tilde{\omega}) = -\alpha_{jk}(\tilde{\omega}). \tag{7–82}
\]
For $\alpha''_{jk}(\tilde{\omega}) = 0$, we must have

$$\tan(\tilde{\omega}) = \frac{x_j - x_k}{y_j - y_k} \frac{Y_j - Y_k}{X_j - X_k}, \quad (7-83)$$

where the last equality is obtained using Equation 7–81. Rewriting we get

$$\left( \frac{Y_j - Y_k}{X_j - X_k} \right)^2 = -1 \quad (7-84)$$

which cannot be true. Since the second derivative cannot vanish at the stationary point $\tilde{\omega}$, from one-dimensional stationary phase approximation [31] we have

$$\lim_{\hbar \to 0} \frac{1}{L^2} \int_{\omega_0}^{\omega_0 + \Delta} \exp \left( -\frac{i\alpha_{jk}(\omega)}{\hbar} \right) \rho_{jk}(\beta, \omega) d\omega = \lim_{\hbar \to 0} O(\hbar^\kappa) = 0 \quad (7-85)$$

where $\kappa = 0.5$ or 1 depending upon whether the interval $[\omega_0, \omega_0 + \Delta)$ contains the stationary point $\tilde{\omega}$ or not. Hence we have $\tau_{jk}(\beta) = 0$ for $j \neq k$.

**Case (ii):** If $j = k$, then $\alpha_{kk}(\omega) = 0$ and

$$\rho_{kk}(\beta, \omega) = \int_{r_k^{(-)}(\beta, \omega)}^{r_k^{(1)}(\beta, \omega)} r' dr', \quad \tau_{kk}(\beta) = \frac{1}{L^2} \int_{\omega_0}^{\omega_0 + \Delta} \rho_{kk}(\beta, \omega) d\omega. \quad (7-86)$$

From the definitions of $r_k^{(1)}(\beta, \omega)$ and $r_k^{(2)}(\beta, \omega)$ in Equation 7–72, observe that

$$\lim_{\beta \to 0} r_k^{(1)}(\beta, \omega) \uparrow R_k^{(1)}(\omega), \quad \lim_{\beta \to 0} r_k^{(2)}(\beta, \omega) \downarrow R_k^{(2)}(\omega). \quad (7-87)$$

Since $r_k^{(-)}(\beta, \omega) \to r_k^{(1)}(\beta, \omega)$ and $r_k^{(+)}(\beta, \omega) \to r_k^{(2)}(\beta, \omega)$ as $\beta \to 0$, we have

$$\lim_{\beta \to 0} r_k^{(-)}(\beta, \omega) = R_k^{(1)}(\omega) \quad \text{and} \quad \lim_{\beta \to 0} r_k^{(+)}(\beta, \omega) = R_k^{(2)}(\omega). \quad (7-88)$$
Since $r_k^-(\beta, \omega) \geq r_k^+(\beta, \omega)$ and $r_k^+(\beta, \omega) \leq r_k^+(\beta, \omega)$ at a fixed $\beta$ and $r' > 0$, we see that $\rho_{kk}(\beta, \omega)$ can be bounded above by positive decreasing function of $\beta$, namely

$$
\rho_{kk}(\beta, \omega) \leq \int_{r_k^+(\beta, \omega)}^{r_k^+(\beta, \omega)} r'dr'
$$

and is also independent of $h$. As both $r_k^+(\beta, \omega)$ and $r_k^+(\beta, \omega)$ are also bounded functions, by the Lesbegue dominated convergence theorem,

$$
\lim_{\beta \to 0} \lim_{h \to 0} \tau_{kk}(\beta) = \frac{1}{L^\epsilon} \int_{\omega_0}^{\omega_0+\Delta} \lim_{\beta \to 0} \rho_{kk}(\beta) d\omega
$$

$$
= \frac{1}{L^\epsilon} \int_{\omega_0}^{\omega_0+\Delta} \left\{ \int_{r_k^+(\omega)}^{r_k^+(\omega)} r'dr' \right\} d\omega
$$

$$
= \frac{(1 - 2\epsilon)}{L^\epsilon} \int_{\omega_0}^{\omega_0+\Delta} \frac{R_k^2(\omega)}{2} d\omega.
$$

Recall that $L^\epsilon = (1 - 2\epsilon)L$. Hence,

$$
\sum_{j=1}^{K} \sum_{k=1}^{K} \lim_{\beta \to 0} \lim_{h \to 0} \tau_{jk}(\beta) = \frac{1}{L} \sum_{k=1}^{K} \int_{\omega_0}^{\omega_0+\Delta} \frac{R_k^2(\omega)}{2} d\omega
$$

$$
= \frac{1}{L} \sum_{k=1}^{K} \int_{\omega_0}^{\omega_0+\Delta} \frac{R_k^2(\omega)}{2} d\omega
$$

$$
= \int_{\omega_0}^{\omega_0+\Delta} P(\omega) d\omega.
$$

which completes the proof. \qed

As an implication of the above theorem, we have the following corollary.

**Corollary 2.** For any given $0 < \delta < 1$, $\omega_0 \in [0, 2\pi)$

$$
\lim_{\epsilon \to 0} \lim_{\Delta \to 0} \frac{1}{\Delta} \lim_{h \to 0} \int_{\omega_0}^{\omega_0+\Delta} \left\{ \int_{1-\delta}^{1+\delta} P_h(r, \omega) d\bar{r} \right\} d\omega = P(\omega_0).
$$

**Proof.** From Equation 7–7 we have

$$
\lim_{\Delta \to 0} \frac{1}{\Delta} \int_{\omega_0}^{\omega_0+\Delta} P(\omega) d\omega = \lim_{\Delta \to 0} \frac{F(\omega_0 \leq \omega \leq \omega_0 + \Delta)}{\Delta} = P(\omega_0).
$$
Since Theorem 7.2 is true for any $0 < \epsilon < \frac{1}{2}$, it also holds good as $\epsilon \to 0$. The result then follows immediately.

Theorem 7.2 also entails the following lemma.

**Lemma 6.** For any given $0 < \epsilon < \frac{1}{2}, 0 < \delta < 1$, 

$$
\lim_{h \to 0} \int_0^{2\pi} \int_{1-\delta}^{1+\delta} P_h^\epsilon(\bar{r}, \omega) \bar{r} d\bar{r} d\omega = 1. \quad (7-94)
$$

**Proof.** Since the result shown in Theorem 7.2 holds good for any $\omega_0$ and $\Delta$, we may choose $\omega_0 = 0$ and $\Delta = 2\pi$. Using Equation 7–8 the result follows immediately as 

$$
\lim_{h \to 0} \int_0^{2\pi} \int_{1-\delta}^{1+\delta} P_h^\epsilon(\bar{r}, \omega) \bar{r} d\bar{r} d\omega = \int_0^{2\pi} P(\omega) d\omega = 1. \quad (7-95)
$$

Lemmas 6 and 5 leads to the following corollaries.

**Corollary 3.** For any given $0 < \epsilon < \frac{1}{2}, 0 < \delta < 1$, 

$$
\lim_{h \to 0} \int_0^{2\pi} \left\{ \int_0^{1-\delta} P_h^\epsilon(\bar{r}, \omega) \bar{r} d\bar{r} + \int_1^{\infty} P_h^\epsilon(\bar{r}, \omega) \bar{r} d\bar{r} \right\} d\omega = 0. \quad (7-96)
$$

**Proof.** From Lemma 5 we have for any $h > 0$ and $0 < \epsilon < \frac{1}{2}$, 

$$
\int_0^{2\pi} \int_0^{\infty} P_h^\epsilon(\bar{r}, \omega) \bar{r} d\bar{r} d\omega = 1. \quad (7-97)
$$

For the given $0 < \delta < 1$, dividing the integral range $(0, \infty)$ for $\bar{r}$ into three disjoint regions namely $(0, 1 - \delta)$, $[1 - \delta, 1 + \delta]$ and $(1 + \delta, \infty)$ and letting $h \to 0$ we have, 

$$
\lim_{h \to 0} \int_0^{2\pi} \left\{ \int_0^{1-\delta} P_h^\epsilon(\bar{r}, \omega) \bar{r} d\bar{r} + \int_{1-\delta}^{1+\delta} P_h^\epsilon(\bar{r}, \omega) \bar{r} d\bar{r} + \int_{1+\delta}^{\infty} P_h^\epsilon(\bar{r}, \omega) \bar{r} d\bar{r} \right\} d\omega = 1. \quad (7-98)
$$

Pursuant to Lemma 6, the limit 

$$
\lim_{h \to 0} \int_0^{2\pi} \int_{1-\delta}^{1+\delta} P_h^\epsilon(\bar{r}, \omega) \bar{r} d\bar{r} d\omega \quad (7-99)
$$

exists and equals 1. The result then follows.
Corollary 4. For any given $0 < \epsilon < \frac{1}{2}$, $0 < \delta < 1$, $\omega_0 \in [0, 2\pi)$ and $0 < \Delta < 2\pi$,

$$\lim_{h \to 0} \int_{\omega_0}^{\omega_0 + \Delta} \left\{ \int_0^{1-\delta} P_h^\epsilon(\tilde{r}, \omega) \tilde{r} d\tilde{r} + \int_{1+\delta}^\infty P_h^\epsilon(\tilde{r}, \omega) \tilde{r} d\tilde{r} \right\} d\omega = 0. \quad (7-100)$$

Proof. Let $M = \left[\frac{2\pi}{\Delta}\right]$. Define $\omega_{i+1} = \omega_i + \Delta \mod 2\pi$ for $0 \leq i \leq M - 1$. Then from Corollary 3 we have

$$\lim_{h \to 0} \sum_{i=0}^{M-1} \int_{\omega_i}^{\omega_{i+1}} Q(\omega) d\omega + \int_{\omega_{i+1}}^{\omega_0 + 2\pi} Q(\omega) d\omega = 0 \quad (7-101)$$

where,

$$Q(\omega) = \int_0^{1-\delta} P_h^\epsilon(\tilde{r}, \omega) \tilde{r} d\tilde{r} + \int_{1+\delta}^\infty P_h^\epsilon(\tilde{r}, \omega) \tilde{r} d\tilde{r}. \quad (7-102)$$

Since $P_h^\epsilon(\tilde{r}, \omega) \tilde{r} \geq 0$, it follows that $Q(\omega)$ and each of the integral in Equation 7–101 is non-negative and hence converges to zero independently of the other integrals, giving

us the desired result.

Pursuant to Theorem 7.2 and Corollaries 2 and 4, the subsequent results follows almost immediately.

Proposition 7.1. For any given $0 < \epsilon < \frac{1}{2}$, $\omega_0 \in [0, 2\pi)$ and $0 < \Delta < 2\pi$,

$$\lim_{h \to 0} \int_{\omega_0}^{\omega_0 + \Delta} \left\{ \int_0^{\infty} P_h^\epsilon(\tilde{r}, \omega) \tilde{r} d\tilde{r} \right\} d\omega = \int_{\omega_0}^{\omega_0 + \Delta} P(\omega) d\omega. \quad (7-103)$$

Corollary 5. For any given $\omega_0 \in [0, 2\pi)$,

$$\lim_{\epsilon \to 0} \lim_{\Delta \to 0} \frac{1}{\Delta} \lim_{h \to 0} \int_{\omega_0}^{\omega_0 + \Delta} \left\{ \int_0^{\infty} P_h^\epsilon(\tilde{r}, \omega) \tilde{r} d\tilde{r} \right\} d\omega = P(\omega_0). \quad (7-104)$$

7.4 Significance of the Result

The integrals

$$\int_{\omega_0}^{\omega_0 + \Delta} \int_{1-\delta}^{1+\delta} P_h^\epsilon(\tilde{r}, \omega) \tilde{r} d\tilde{r} d\omega, \quad \int_{\omega_0}^{\omega_0 + \Delta} P(\omega) d\omega \quad (7-105)$$
gives the interval measure of the density functions \( P_h \) (when polled close to the unit circle \( \tilde{r} = 1 \)) and \( P \) respectively. Theorem 7.2 states that at small values of \( h \), both the interval measures are approximately equal, with the difference between them being \( o(1) \). Furthermore the result is also true as \( \epsilon \to 0 \). Recall that by definition \( P_h^c \) is the normalized power spectrum of the wave function \( \phi(x, y) = \exp \left( \frac{iS(x, y)}{\hbar} \right) \). Hence we conclude that the power spectrum of \( \phi(x, y) \) when polled close to the unit circle \( \tilde{r} = 1 \) (as \( \delta \to 0 \) in Theorem 7.2) or when integrated over \( \tilde{r} \) (refer Proposition 7.1), can potentially serve as a density estimator for the orientation density of \( S \) at small values of \( \hbar \) and \( \epsilon \). The empirical results shown under Section 8.5 also provide visual evidences to corroborate to our claim.
CHAPTER 8
EXPERIMENTAL RESULTS

In Section 5.3.1 we gave an account on the numerical issues involved in computing the wave function $\phi$ and the need for arbitrary precision arithmetic packages like GMP and MPFR [20, 45] in floating-point computations. For the following experiments on Euclidean distance functions and eikonal equations, we we used $p = 512$ precision bits.

8.1 Euclidean Distance Functions

In this section, we show the efficacy of our Schrödinger method by computing the approximate Euclidean distance function $S$ and comparing it to the actual Euclidean distance function and the fast sweeping method, first on randomly generated 2D point-sets and then on a set of bounded 2D and 3D grid points.

8.1.1 2D Experiments

Example 1: We begin by demonstrating the effect of $h$ on our Schrödinger method and show that as $h \to 0$, the accuracy our method does improve significantly. To this end, we considered a 2D grid consisting of points between $(-0.121, -0.121)$ and $(0.121, 0.121)$ with a grid width of $\frac{1}{2^9}$. The total number of grid points is then $N = 125 \times 125 = 15,625$. We ran 1000 experiments each time randomly choosing 5000 grid locations as data points (point-set), for 9 different values of $h$ ranging from $5 \times 10^{-5}$ to $4.5 \times 10^{-4}$ in steps of $5 \times 10^{-5}$. For each run and each value of $h$, we calculated the percentage error as

$$error = \frac{100}{N} \sum_{i=1}^{N} \frac{\Delta_i}{D_i},$$

where $D_i$ and $\Delta_i$ are respectively the actual distance and the absolute difference of the computed distance to the actual distance at the $i^{th}$ grid point. The plot in Figure 8-1 shows the mean percentage error at each value of $h$. The maximum value of the error at each value of $h$ is summarized in Table 8-1. The error is less than 0.6% at $h = 0.00005$ demonstrating the algorithm’s ability to compute accurate Euclidean distances.
Table 8-1. Maximum percentage error for different values of $\tilde{h}$ in 1000 2D experiments.

<table>
<thead>
<tr>
<th>$\tilde{h}$</th>
<th>Maximum percentage error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00005</td>
<td>0.5728%</td>
</tr>
<tr>
<td>0.00010</td>
<td>1.1482%</td>
</tr>
<tr>
<td>0.00015</td>
<td>1.7461%</td>
</tr>
<tr>
<td>0.00020</td>
<td>2.4046%</td>
</tr>
<tr>
<td>0.00025</td>
<td>3.1550%</td>
</tr>
<tr>
<td>0.00030</td>
<td>4.0146%</td>
</tr>
<tr>
<td>0.00035</td>
<td>4.9959%</td>
</tr>
<tr>
<td>0.00040</td>
<td>6.1033%</td>
</tr>
<tr>
<td>0.00045</td>
<td>7.3380%</td>
</tr>
</tbody>
</table>

**Example 2:** We pitted the Schrödinger algorithm against the fast sweeping method [50] on a 2D grid consisting of points between $(-0.123, -0.123)$ and $(0.123, 0.123)$ with the grid with of $\frac{1}{2n}$. The number of grid points equals $N = 253 \times 253 = 64,009$. We ran 100 experiments, each time randomly choosing 10,000 grid points as data points. We set $\tilde{h} = 0.0001$ for the Schrödinger and ran the fast sweeping for 10 iterations sufficient for it to converge. The plot in Figure 8-2 shows the average percentage error calculated according to Equation 8–1 for both these techniques in comparison to the true Euclidean distance function. From the plot, it is clear that while the fast sweeping method has a percentage error of around 7%, Schrödinger method gave a percentage error of less than 1.5% providing much better accuracy.
Example 3: In this example, we computed the Euclidean distance transform using the grid points of certain silhouettes (Figure 8-3) [42], on a 2D grid consisting of points between \((-0.125, -0.125)\) to \((0.125, 0.125)\) with a grid width of \(\frac{1}{2}\). The number of grid points equals \(N = 257 \times 257 = 66049\). We set \(h\) for the Schrödinger method 0.0003. For the sake of comparison, we ran the fast sweeping for 10 iterations which was sufficient for convergence. The percentage error for the Schrödinger and the fast sweeping (calculated as per Equation 8–1 when compared with the true Euclidean distance function for each of these shapes is adumbrated in Table 8-2.

---

1 We thank Kaleem Siddiqi for providing us the set of 2D shape silhouettes.
Table 8-2. Percentage error of the Euclidean distance function computed using the grid points of the shapes as data points

<table>
<thead>
<tr>
<th>Shape</th>
<th>Schrödinger</th>
<th>Fast sweeping</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hand</td>
<td>2.182%</td>
<td>2.572%</td>
</tr>
<tr>
<td>Horse</td>
<td>2.597%</td>
<td>2.549%</td>
</tr>
<tr>
<td>Bird</td>
<td>2.116%</td>
<td>2.347%</td>
</tr>
</tbody>
</table>

The true Euclidean distance function contour plot and those obtained from our method and fast sweeping is delineated in Figure 8-4.

![Figure 8-4. Shape contour plots. A) True Euclidean distance function. B) Schrödinger. C) Fast sweeping.](image)

8.1.2 Medial axis computations

In order to compute the medial axis for these shapes, we first need to differentiate between the grid locations that are either inside or outside of each shape. We did it by computing the winding number for all the grid points simultaneously using our convolution based winding number algorithm. Grid points with a winding number value
of greater than zero after round off where marked as interior points and rest were marked as exterior points. Figure 8-5 visualizes the vector fields \((S_x, S_y)\) for all the interior points (marked in blue) and the exterior points (marked in red). Clearly we see that our convolution based technique for computing the winding number cleanly (with almost zero error) separated the inside grid points from those that are exterior to the 2D shape.

Figure 8-5. A quiver plot of \(\nabla S = (S_x, S_y)\) (best viewed in color).

We chose the maximum curvature (defined as \(H + \sqrt{H^2 - K}\) where \(H\) and \(K\) are the mean and Gaussian curvatures respectively of the Monge patch given by \(\{x, y, S(x, y)\}\)) as the vehicle to visualize the medial axis of each shape. The mean
and Gaussian curvatures can be expressed in terms of the coefficients of the first and second fundamental forms \((E, F, G\) and \(e, f, g\) [23]) respectively which are in turn expressible in closed-form using the first and second derivatives of \(S\). As these derivatives can be written as discrete convolutions (elucidated in Section 4.3), the max-curvature for the Monge patch can be computed in \(O(N \log N)\) using FFT. From the max-curvature we can easily retrieve the medial axis as explained below.

Observe from the quiver plots in Figure 8-5, that the gradient directions are preserved until they meet with the gradients emanating from other curve locations. A zoomed version of the quiver plot is shown in Figure 8-6. In places where the gradients meet, their directions change significantly and hence the surface \(S(x, y)\) exhibits high max-curvature values at those locations. But these locations exactly correspond to the grid points having more than one closest point on the shape’s boundary–also known as the Voronoi boundary points or the medial axis points. Hence a simple thresholding of the max-curvature gives the medial axis, as determined by the points where the max-curvature is greater than (say) \(\tau_1\). The medial axis plots for these shapes are shown in Figure 8-7 and can also be easily traced from the quiver plots (Figure 8-5) when viewed in color.

Figure 8-6. Zoomed quiver plot
We would like to mention that, computing the medial axis using the max-curvature is handicapped by a minor drawback. Using FFT to compute the distance transform and its derivatives, forces the data to sit on a regular grid. Notice from the medial axis plots (Figure 8-7) that the boundary of these shapes are not smooth but rugged. This resulted in high max-curvature values at various spurious locations, especially at the grid locations which are very close to the boundary points \( Y_k \) and hence will also be labelled as points on the medial axis. To circumvent this, we incorporated a second level of thresholding whereby we consider only those grid locations \( X \) where the distance transform \( S(X) \) is greater than (say) \( \tau_2 \). Depending on the shape, \( \tau_1 \) was set between 0.09 and 0.12 and \( \tau_2 \) between 3\( \delta \) and 6\( \delta \) where \( \delta = 1/2^{10} \) is the grid width.

An easier fix to the aforementioned problem is to run our method on a much finer grid, increasing the number of grid locations and having a smooth boundary. But this has an adverse effect of slowing down the running time. A better solution would be to adapt the grid depending upon the data with varying grid width for different locations. Extending our technique for irregular grids is beyond the scope of our current work. We would like to address this in our future work.

### 8.1.3 3D Experiments

**Example 4:** We took the Stanford bunny dataset\(^2\) and used the coordinates of the data points on the model as our point-set locations. Since the input data locations need not conform to grid locations, we scaled the space uniformly in all dimensions and rounded off the data so that the data lies at grid locations. The input data was also shifted so that it was approximately symmetrically located with respect to the \( x, y \) and \( z \) axis. We should point out that shifting the data doesn’t affect the Euclidean distance function value and uniform scaling of all dimensions is also not an issue, as the distances can be

\(^2\) This dataset is available at [http://www.cc.gatech.edu/projects/large_models/bunny.html](http://www.cc.gatech.edu/projects/large_models/bunny.html)
rescaled after they are computed. Moreover, the formula for calculating the percentage error (Equation 8–1) is invariant to shifting and scaling.

After these basic data manipulations, the cardinality of the point set was $K = 8948$ with the data confined to the cubic region $-0.117 \leq x \leq 0.117, -0.117 \leq y \leq 0.117$ and $-0.093 \leq z \leq 0.093$, with a grid width of $\frac{1}{2h}$. The number of points on the grid equals $N = 182,329$. We ran the Schrödinger with $\hbar = 0.0004$ and the Fast sweeping for 15 iterations and later calculated the percentage error for both these methods by comparing with the true distance function according to Equation 8–1. Our method had a percentage error of only 1.23% and favorably compares to fast sweeping which had
a percentage error of 4.75%. Our FFT-based approach does not begin by discretizing the spatial differential operator as is the case with the fast marching and fast sweeping methods and this could help account for the increased accuracy.

The isosurface obtained by connecting the grid points at a distance of 0.005 from the point set, determined by the true Euclidean distance function, Schrödinger and the fast sweeping is shown in Figure 8-8. Notice the similarity between the plots. It provides anecdotal visual evidence for the usefulness of our approach.

![Figure 8-8. Bunny isosurfaces. A) Actual Euclidean distance function. B) Schrödinger. C) Fast sweeping.](image)

**Example 5:** We also compared the Schrödinger Euclidean distance function algorithm with the fast sweeping method [50] and the exact Euclidean distance on the Dragon point-set obtained from the Stanford 3D Scanning Repository ³. After the initial shifting, scaling and rounding of the data points so that they conform to grid locations, the common grid for this data set was $-0.117 \leq x \leq 0.117, -0.086 \leq y \leq 0.086$ and $-0.047 \leq z \leq 0.047$ with a grid width of $\frac{1}{256}$. We ran the Schrödinger approach at $\delta = 0.0004$ and ran the fast sweeping method for 15 iterations sufficient for the Gauss-Seidel iterations to converge. We then calculated the percentage error as per

³ This dataset is available at [http://graphics.stanford.edu/data/3Dscanrep/](http://graphics.stanford.edu/data/3Dscanrep/).
Equation 8–1. While the average percentage error in the Schrödinger approach when compared to the true distance function was just 1.306%, the average percentage error in the fast sweeping method was 6.84%.

The isosurface obtained by connecting the grid points at a distance of 0.005 from the point set, determined by the true Euclidean distance function, Schrödinger and fast sweeping are shown in Figure 8-9. The similarity between the plots provides anecdotal visual evidence for the usefulness of our approach.

![Figure 8-9. Dragon isosurfaces. A) Actual Euclidean distance function. B) Schrödinger. C) Fast sweeping.](image)

### 8.2 The General Eikonal Equation

In this section we demonstrate the usefulness of our approach by computing the approximate solution to the general eikonal equation over a regular 2D grid.

#### 8.2.1 Comparison with the True Solution

**Example 6:** In this example, we solve the eikonal equation for the scenario where the exact solution is known a priori at the grid locations. The exact solution is

\[
S(x, y) = |e^{\sqrt{x^2+y^2}} - 1|.
\]

The boundary condition is, \(S(x, y) = 0\) at the point source located at \((x_0, y_0) = (0, 0)\).

The forcing function—the absolute gradient \(|\nabla S|\)—is

\[
f(x, y) = |\nabla S| = e^{\sqrt{x^2+y^2}}
\]

(8–3)
specified on a 2D grid consisting of points between \((-0.125, -0.125)\) and \((0.125, 0.125)\) with a grid width of \(\frac{1}{2^{10}}\). We ran the Schrödinger for 6 iterations at \(h = 0.006\) and the fast sweeping for 15 iterations sufficient enough for both the methods to converge. The percentage error (calculated according to Equation 8–1) and the maximum difference between the true and approximate solution for different iterations is summarized in the Table 8-3.

Table 8-3. Percentage error and the maximum difference for the Schrödinger method over different iterations

<table>
<thead>
<tr>
<th>Iter</th>
<th>Percentage error</th>
<th>Max difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.081042</td>
<td>0.002651</td>
</tr>
<tr>
<td>2</td>
<td>1.514745</td>
<td>0.002140</td>
</tr>
<tr>
<td>3</td>
<td>1.390552</td>
<td>0.002142</td>
</tr>
<tr>
<td>4</td>
<td>1.363256</td>
<td>0.002128</td>
</tr>
<tr>
<td>5</td>
<td>1.357894</td>
<td>0.002128</td>
</tr>
<tr>
<td>6</td>
<td>1.356898</td>
<td>0.002128</td>
</tr>
</tbody>
</table>

The fast sweeping gave a percentage error of 1.135\%. We believe that the error incurred in our Schrödinger approach can be further reduced by decreasing \(h\) but at the expense of more computational power requiring higher precision floating point arithmetic.

The contour plots of the true solution and those obtained from Schrödinger and fast sweeping are displayed below (Figure 8-10). We can immediately observe the similarity of our solution with the true solution. We do observe smoother isocontours in our Schrödinger method relative to fast sweeping.

Figure 8-10. Contour plots. A) True solution. B) Schrödinger. C) Fast sweeping
8.2.2 Comparison with Fast Sweeping

In order to verify the accuracy of our technique, we compared our solution with fast sweeping for the following set of examples, using the latter as the ground truth as the true solution is not available in closed-form.

**Example 7:** In this example we solved the eikonal equation from a point source located at \((x_0, y_0) = (0, 0)\) for the following forcing function

\[
f(x, y) = 1 + 2(e^{-2((x+0.05)^2+(y+0.05)^2)} - e^{-2((x-0.05)^2+(y-0.05)^2)})
\]

(8–4)

on a 2D grid consisting of points between \((-0.125, -0.125)\) and \((0.125, 0.125)\) with a grid width of \(\frac{1}{2^m}\). We ran our method for 6 iterations with \(h\) set at 0.015 and fast sweeping for 15 iterations sufficient for both techniques to converge. When we calculated the percentage error for the Schrödinger according to Equation 8–1 (with fast sweeping as the ground truth), the error was just around 1.245\%. The percentage error and maximum difference between the fast sweeping and Schrödinger solutions after each iteration are adumbrated in Table 8-4.

Table 8-4. Percentage error and the maximum difference for the Schrödinger method in comparison to fast sweeping

<table>
<thead>
<tr>
<th>Iter</th>
<th>Percentage error</th>
<th>Max difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.144632</td>
<td>0.008694</td>
</tr>
<tr>
<td>2</td>
<td>1.269028</td>
<td>0.008274</td>
</tr>
<tr>
<td>3</td>
<td>1.223836</td>
<td>0.005799</td>
</tr>
<tr>
<td>4</td>
<td>1.246392</td>
<td>0.006560</td>
</tr>
<tr>
<td>5</td>
<td>1.244885</td>
<td>0.006365</td>
</tr>
<tr>
<td>6</td>
<td>1.245999</td>
<td>0.006413</td>
</tr>
</tbody>
</table>

We believe that the fluctuations both in the percentage error and the maximum difference are due to repeated approximations of the integration involved in the convolution with discrete convolution and summation, but nevertheless stabilized after 6 iterations. The contour plots shown in Figure 8-11 clearly demonstrate the similarities between these methods.
Example 8: Here we solved the eikonal equation for the sinusoidal forcing function

\[ f(x, y) = 1 + \sin(\pi(x - 0.05)) \sin(\pi(y + 0.05)) \]  

(8–5)

on the same 2D grid as in the previous example. We randomly chose 4 grid locations namely,

\[ \{0, 0\}, \{0.0488, 0.0977\}, \{-0.0244, -0.0732\}, \{0.0293, -0.0391\} \]

as data locations and ran our method for 6 iterations with \( \bar{h} \) set at 0.0085 and ran fast sweeping for 15 iterations. The percentage error between the Schrödinger solution (after 6 iterations) and fast sweeping was 4.537% with the maximum absolute difference between them being 0.0109.

The contour plots are shown in Figure 8-12. Notice that the Schrödinger contours are more smoother in comparison to the fast sweeping contours.

Figure 8-12. Contour plots. A) Schrödinger. B) Fast sweeping.
Example 9: Here we compared with fast sweeping on a larger 2D grid consisting of points between \((-5, -5)\) and \((5, 5)\) with a grid width of 0.25. We again considered the sinusoidal forcing function

\[
f(x, y) = 1 + 0.3 \sin(\pi(x + 1)) \sin(\pi(y - 2))
\]  

(8–6)

and chose 4 grid locations namely \(\{0, 0\}, \{1, 1\}, \{-2, -3\}, \{3, -4\}\) as data locations. Notice that the Green’s function \(G\) and \(\tilde{G}\) goes to zero exponentially faster for grid locations away from zero for small values of \(h\). Hence for a grid location say \((-4, 4)\) which is reasonably far away from 0, the value of the Green’s function say at \(h = 0.001\) may be zero even when we use a large number of precision bits \(p\). This problem can be easily circumvented by first scaling down the entire grid by a factor \(\tau\), computing the solution \(S^*\) on the smaller denser grid and then rescaling it back again by \(\tau\) to obtain the actual solution. It is worth emphasizing that scaling down the grid is tantamount to scaling down the forcing function as clearly seen from the fast sweeping method.

In fast sweeping [50], the solution \(S^*\) is computed using the quantity \(f_{i,j}\delta\) where \(f_{i,j}\) is the value of forcing function at the \((i,j)^{th}\) grid location and \(\delta\) is the grid width. Hence scaling down \(\delta\) by a factor of \(\tau\) is equivalent to fixing \(\delta\) and scaling down \(f\) by \(\tau\). Since the eikonal equation (Equation 1–1) is linear in \(f\), computing the solution for a scaled down \(f\)–equivalent to a scaled down grid–and then rescaling it back again is guaranteed to give the actual solution.

\(\tau\) can be set to any desired quantity. For the current experiment we set \(\tau = 100\), \(h = 0.001\) and ran our method for 6 iterations. Fast sweeping was run for 15 iterations. The percentage error between these methods was about 3.165%. The contour plots are shown in Figure 8-13. Again, the contours obtained from the Schrödinger are more smoother than those obtained from fast sweeping.
8.3 Topological Degree Experiments

We demonstrated the efficacy of our convolution based technique for computing the winding number in 2D, when we computed the medial axis for the silhouettes. We now show its accuracy for computing the topological degree in 3D. To this end, we considered a 3D grid, confined to the region $-0.125 \leq x \leq 0.125$, $-0.125 \leq y \leq 0.125$ and $-0.125 \leq z \leq 0.125$ with a grid width of $\frac{1}{2^8}$. The number of grid points was $N = 274,625$. Given a set of points sampled from the surface of a 3D object, we triangulated the surface using some of the built-in MATLAB routines. We considered the incenter of each triangle to represent the data points $\{Y_k\}_{k=1}^K$. The normal $P_k$ for each triangle can be computed from the cross product of the triangle vector edges. The direction of the normal vector was determined by taking the dot product between the position vector $Y_k$ and the normal vector $P_k$. For negative dot products, $P_k$ was negated to obtain a outward pointing normal vector. We then computed the topological degree for all the $N$ grid locations simultaneously by running our convolution based algorithm. Grid locations where the topological degree value exceeded 0.7 were marked as points lying inside the given 3D object. Figure 8-14 shows the interior points for the three 3D objects cylinder, cube and sphere (left to right).
Figure 8-14. Topological Degree. A) Sampled points from the surface. B) Grid points lying inside the surface (marked in blue).

8.4 Empirical Results for the Gradient Density estimation in One Dimension

Below we show comparisons between our Fourier transform approach with the standard histogramming technique for estimating the gradient densities on some trigonometric and exponential functions sampled on a regular grid between \([-0.125, 0.125]\) at a grid spacing of \(\frac{1}{2^{15}}\). For the sake of convenience, we normalized the functions such that its maximum gradient value is 1. Using the sampled values \(\hat{S}\), we computed the Fast Fourier transform of \(\exp \left( \frac{i \hat{S}}{h} \right)\) at \(h = 0.00001\), took its magnitude
square and then normalized it to compute the gradient density. We also computed the
discrete derivative of $S$ at the grid locations and then determined its gradient density
using the standard histogramming technique with 220 histogram bins. The plots shown
in Figure 8-15 provide anecdotal empirical evidence, supporting the mathematical result
stated in Theorem 6.1 under Chapter 6. Notice the near-perfect match between the
gradient densities computed via standard histogramming, with the gradient densities
determined using our Fourier transform method.

![Figure 8-15. Comparison results. A) Gradient densities obtained from histogramming. B) Gradient densities obtained from squared Fourier transform of the wave function](image)

8.5 Empirical Results for the Density Functions of the Distance Transforms

8.5.1 CWR and its Fourier Transform

On the left side of the Figure 8-16 and Figure 8-16, we visualize the CWR of the
distance transform $S$, computed earlier for some of these shape silhouettes. Since the
wave function $\phi = \exp \left( \frac{iS}{\lambda} \right)$ has both the real and the imaginary part, we show only
its imaginary component, namely $\sin \left( \frac{iS}{\lambda} \right)$ for visual clarity. Using these plots we can
envisage a wave emanating from the boundaries of these shapes (represented by thick black lines). These CWR plots were computed at $\hbar = 0.5$.

On the right side of the Figure 8-16 and Figure 8-16, we plot the Fourier transform of $\phi$ at $\hbar = 0.00004$. We see a bright blue segment defined only on the unit circle $u^2 + v^2 = r^2 = 1$, over a plain, non-interesting, flat background. The shades of blue represents the variation in the magnitude of the Fourier transform. While the bright blue regions represents high values in the magnitude, the non-bright, flat regions corresponds to very low, almost zero magnitude value.

Theorem 7.1 given under Section 7.2 states that "Expect on the unit circle given by $\tilde{r} = 1$, the Fourier transform of the wave function should converge to zero as $\hbar \to 0$". These pictures exactly portrays the theorem statement. Except on the unit circle $\tilde{r} = 1$ where we observe high values, the magnitude of the Fourier transform is almost zero everywhere else.

8.5.2 Comparison Results

Below we show equivalence between our Fourier transform approach and the true orientation density of the unit vector distance transform gradients, determined using the closed-form expression derived in Equation 7–7. Using the sampled values $\hat{S}$, sampled on the given 2D grid $-0.125 \leq x \leq 0.125, -0.125 \leq y \leq 0.125$ at intervals of $\frac{1}{256}$, we computed the Fast Fourier transform of $\exp \left( \frac{i \hat{S}}{\hbar} \right)$ at $\hbar = 0.000004$. We then shifted the frequencies, so that the zero-frequency component is in the middle of the spectrum and then took its magnitude square to compute the discrete power spectrum. Using 140 histogram bins for the angle $\omega$, we summed up the power spectrum values along discrete radial directions (analogous to integrating over $\tilde{r}$) and renormalized it in order to compute the orientation density function. Notice the similarities between the plots shown in Figure 8-17.
Furthermore at each value of $\tilde{h}$, we computed the $L_1$ error between the true and the computed density function, by computing the absolute difference between their values at each histogram bin and then adding up the differences. From the two plots shown in Figure 8-18, we can visualize the convergence of $L_1$ error to zero as $\tilde{h} \to 0$. These plots serve as a testament, strengthening our mathematical result stated under Theorem 7.1.
Figure 8-16. Continued
Figure 8-17. Comparison results. A) True gradient density function. B) Gradient density function obtained from the squared Fourier transform of the CWR.

Figure 8-18. Plot of $L_1$ error vs $h_i$ for the orientation density functions.
CHAPTER 9
DISCUSSION AND FUTURE WORK

9.1 Conclusion

In this work, we provided an application of the Schrödinger formalism where we developed a new approach to solving the non-linear eikonal equation. We proved that the solution to the eikonal equation can be obtained as a limiting case of the solution to a corresponding linear Schrödinger wave equation. Instead of directly solving the eikonal equation, the Schrödinger formalism results in a generalized, screened Poisson equation which is solved at very small values of $\hbar$. Our Schrödinger-based approach follows the pioneering Hamilton-Jacobi solvers such as the fast sweeping [50] and fast marching [34] methods with the crucial difference being its linearity. We developed a fast and efficient perturbation series method for solving the wave equation (generalized, screened Poisson equation) which is guaranteed to converge provided the forcing function $f$ is positive and bounded. Using the perturbation method and the Equation 2–51, we obtained the solution to the Equation 2–49 without spatially discretizing the operators.

For the Euclidean function problem—a special case of the eikonal equation where the forcing term is identically equal to one everywhere—we obtained closed-form solutions for the Schrödinger wave equation that can be efficiently computed using the FFT which involves $O(N \log N)$ floating-point operations. The Euclidean distance is then recovered from the exponent of the wave function. Since the wave function is computed for a small but non-zero $\hbar$, the obtained Euclidean distance function is an approximation. We derived analytic bounds for the error of the approximation for a given value of $\hbar$ and provided proofs of convergence to the true distance function as $\hbar \to 0$. We then leveraged the differentiability of the Schrödinger solution to compute the gradients and curvature of the distance function $S$, by giving a closed-form expression which can be written as convolutions. We also provided an efficient mechanism to determine the sign
of the distance function with our discrete convolution based technique for computing the winding number in 2D and the topological degree in 3D and showed how the gradient and curvature information can aid in medical axes computation, when applied to 2D shape silhouettes.

Our results on density estimation, directly inspired by momentum density in quantum mechanics, demonstrates the usefulness of theoretical physics ideas in contexts of density estimation. Using stationary phase approximations we established that the scaled power spectrum of the wave function approaches the density of the gradient(s) of the distance function \( S \) in the limit as \( \hbar \to 0 \), when the scalar field \( S \) appears as the phase of the wave function. By providing rigorous mathematical proofs, we established this relation between the gradients and the frequencies for an arbitrary thrice differentiable function in one dimension and specifically for distance transforms in two dimension. We also furnished anecdotal visual evidences to corroborate our claim. Our result gives a new signature for the distance transforms and can potentially serve as its gradient density estimator.

9.2 Future Work

While Hamilton-Jacobi solvers have gone beyond the eikonal equation and regular grids—by providing efficient solutions even for the more general static Hamilton-Jacobi equation on irregular grids [26, 27, 36]—our Schrödinger approach in the current work restricts itself only to computing the eikonal equation on regular grids. Since our method relies on using Fast Fourier Transform (FFT’s) for computation, we were restricted to define the data only on regular grid locations. However, recently developed non-FFT based techniques like the fast multipole methods might pave the way to extend our Schrödinger formalism even for irregular grids.

In our current work, we established the mathematical relation between the power spectrum of the wave function and its gradient densities only for distance transforms. But preliminary experimental results seems to suggest that the result is generalizable to
a more general class of functions with appropriate boundary conditions. We would like to investigate this further and if it pans out, try to support our empirical discovery with rigorous mathematical proofs. This represents a fruitful avenue for future research.
REFERENCES


BIOGRAPHICAL SKETCH

Karthik S. Gurumoorthy hails from the southern part of India, from the city of Madras (now called Chennai). After completing his baccalaureate degree in computer engineering from the University of Madras in 2004, he worked for an year as a software developer at HCL-cisco, Chennai. Having a penchant for mathematics and research, he decided to pursue higher education and got admitted for a Ph.D. program in computer engineering at University of Florida (UF) in 2005. Amid continuing with his Ph.D., he concurrently signed up for a dual master’s program in mathematics at UF and earned M.S in mathematics in the year 2009. He also received his M.S in computer science in 2010. His primary research interest is in developing computationally efficient techniques with inspiration from quantum mechanics, exploiting the known relationship between the classical Hamilton-Jacobi equation and the quantum Schrödinger equation to solve well known classical problems like the eikonal equation, estimation of the the gradient densities, etc. He has also worked in the field of sparse representations, compressibility of sets through the repeated iteration of a polynomial function and in 2-worker bucket-brigade lines.