A Classical Perspective on Non-Diffractive Disorder

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A Classical Perspective on Non-Diffractive Disorder

A DISSERTATION PRESENTED
BY
ANNA MARGARET KLALES
TO
THE DEPARTMENT OF PHYSICS

IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
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A Classical Perspective on Non-Diffractive Disorder

ABSTRACT

The unifying themes connecting the chapters in this dissertation are the profound and often surprising effects of disorder in classical and quantum systems and the tremendous insight gained from a classical perspective, even in quantum systems. In particular, we investigate disorder in the form of weak, spatially correlated random potentials, i.e. far from the Anderson Localization regime.

We present a new scar-like phenomenon in quantum wells. With the introduction of local impurities to the oscillator, the eigenstates localize onto classical periodic orbits of the unperturbed system. Compared to traditional scars in chaotic billiards, these scars are both more common and stronger. Though the unperturbed system has circular symmetry, the random perturbation selects a small number of orientations which are shared by many scarred states – dozens or even hundreds – over a range of energies. We show, via degenerate perturbation theory, that the cause of the new scars is the combination of an underlying classical resonance of the unperturbed system and a perturbation induced coupling that is strongly local in action space.

Next we examine the same type of local perturbation applied to an open system: branched flow. Caustics in the manifold of trajectories have been implicated in the formation of strong branches. We show that caustic formation is intimately tied to compression of manifolds of trajectories in phase space, which has important implications for the position space density. We introduce the “Kick and Drift” model, a generalization of the standard map. The model is a good approximation to the full two dimensional dynamics of a wave propagating over a weak random potential, but it provides a simpler framework for studying branched flow.

Next we develop a classical model for electrons executing cyclotron motion in a graphene flake and implement it numerically. We derive classical equations of motion for electrons moving through the graphene flake with a position dependent effective mass due to fluctuations in the background carrier density. I apply these methods
to an experiment performed by the Westervelt group. They imaged the flow of electrons in a graphene flake by measuring the transresistance as they rastered a charged scanning probe microscope tip over the surface. My simulations show that the regions with the greatest change in transresistance do always coincide with the regions with the highest current density. Furthermore I show that the experimental results can qualitatively reproduced by treating the system classically.

Finally, we extend Heller’s thawed Gaussian approximation from second order in the classical action to third order, in order to capture curvature in phase space. Such phase space dynamics are ubiquitous in systems with weak random potentials, such as those discussed above. We derive a closed form solution, but find that more work needs to be done to make it numerically tractable and competitive with other methods. A semiclassical method capturing phase space curvature could provide insight into the behavior of scars away from the $\hbar \to 0$ limit.
1 NEAR-DEGENERACY IN NOISY OSCILLATORS .......................................................... 1
  1.1 Traditional scar theory ....................................................................................... 4
  1.2 New scars ........................................................................................................... 9
  1.3 Single impurity $r^5$ case .................................................................................... 9
  1.4 The degenerate harmonic oscillator with random Gaussian perturbations ............ 11
  1.5 The $r^5$ oscillator ............................................................................................. 15
  1.6 Performance of degenerate perturbation theory .................................................. 23
  1.7 Conclusion .......................................................................................................... 29

2 THE KICK AND DRIFT MODEL ........................................................................... 31
  2.1 Introduction ......................................................................................................... 31
  2.2 A single caustic ................................................................................................... 35
  2.3 The kick and drift model ...................................................................................... 37
  2.4 The effect of phase space dynamics on manifold slope ........................................... 40
  2.5 The effect of phase space dynamics on manifold stretching .................................... 42
  2.6 The rarefaction exponent .................................................................................... 44
  2.7 Critical Slope ....................................................................................................... 47
  2.8 Evolution of the slope ........................................................................................ 48
  2.9 Rarefaction ......................................................................................................... 50
  2.10 Curvature .......................................................................................................... 52
  2.11 Periodic branched flow ...................................................................................... 55

3 MAGNETIC FOCUSING IN GRAPHENE ............................................................... 60
  3.1 The experiment .................................................................................................... 61
  3.2 Theory ................................................................................................................ 63
  3.3 Experimental geometry ...................................................................................... 67
  3.4 The simulation .................................................................................................... 68
  3.5 Results ................................................................................................................. 73
3.6 Interpreting the image ................................................. 75
3.7 Discussion ............................................................... 82
3.8 Conclusion ............................................................... 83

4 THIRD ORDER THAWED GAUSSIAN APPROXIMATION 84
   4.1 Thawed Gaussian Approximation ................................. 86
   4.2 The third order expansion ......................................... 86
   4.3 Closed-Form Solution .............................................. 88
   4.4 Computation .......................................................... 92
   4.5 Classical behavior ................................................... 95

REFERENCES 100
Listing of figures

1.1 Sample array of eigenstates in the perturbed system. .......................... 2
1.2 Autocorrelation of Gaussian wavepacket launched in a quartic potential. 5
1.3 Fourier transform of autocorrelation of Gaussian wavepacket launched in a quartic potential. .................................................. 6
1.4 States of the degenerate 2:1 oscillator with perturbation .................... 13
1.5 Mixing with perturbation ............................................................... 14
1.6 Almost 1:1 oscillator ........................................................................ 16
1.7 Resonant sets ................................................................................... 17
1.8 Coupling matrix ............................................................................... 20
1.9 States calculated via degenerate perturbation theory on a small subset of states within a resonant set. ...................................................... 24
1.10 States calculated (almost) exactly via diagonalization on a very large subset of basis states. ............................................................... 25
1.11 The perturbing potentials ................................................................. 26
1.12 DPT vs. exact eigenstates ................................................................. 27
1.13 Eigenstates of a the non-degenerate harmonic oscillator. ............... 28
1.14 Short figure name. ............................................................................ 29

2.1 Phase space manifold projection......................................................... 33
2.2 Basic caustic formation ..................................................................... 34
2.3 Dot density evolution. ....................................................................... 36
2.4 Full 2D branched flow simulation ..................................................... 39
2.5 Kick and drift results ....................................................................... 39
2.6 Effect of a shear on slope. ................................................................. 41
2.7 Manifold compression in phase space. ........................................... 45
2.8 Rarefaction along a trajectory. .......................................................... 46
2.9 Distribution of compression at caustics. ......................................... 46
2.10 Three infinitessimally spaced points. .............................................. 53
2.11 Three evolved infinitessimally spaced points.
2.12 Classical periodic branched flow
2.13 Quantum periodic branched flow
2.14 Quantum-classical correspondence in branched flow.

3.1 Graphene sample connected to leads. $R = 10M\Omega$.
3.2 Ideal point source and drain
3.3 These are two-dimensional spatial histograms only of trajectories that make it from Lead 1 to Lead 3. The contacts here are only 200 nm wide.
3.4 Theoretical electron flow without tip
3.5 These are plots only of trajectories that make it from Lead 1 to Lead 3.
3.6 Experimental field of view
3.7 Simulation results with large tip
3.8 Results with mean free path
3.9 Theoretical electron flow with tip.
3.10 Trajectory density contributing to current measured with tip.

4.1 First overlap.
In loving memory of William Frank McClune.
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A new type of scar was discovered by our collaborators, Perttu J. J. Luukko and Esa Räsänen, using their open source imaginary time propagation code, \texttt{itp2d}\textsuperscript{21} in noisy quintic potentials\textsuperscript{20}. The open source code they developed allowed them to calculate several thousand of the lowest energy states. The eigenfunctions demonstrate striking behavior; many of them are scarred with five-pointed stars, but there are also bouncing ball scars, seven-pointed stars, nine-pointed stars, etc. A sampling of these, created with code written by B. Drury, is shown in Figure 1.1. Furthermore, the stars are consistently oriented in only a few directions over a fairly large range of energies. In this section, I'll discuss the observations made of these scars and the theoretical
Figure 1.1: An array of eigenstates with consecutive energies in the noisy quintic potential. The preferred orientations of the states can be seen in this array.
work I did to explain their origin and why they assume particular orientations.

Since the discovery of scars\textsuperscript{12}, scarring has been observed in many experimental systems. The first scar was observed experimentally in the mid-nineties - an electronic state confined in a semiconductor well with a high magnetic field\textsuperscript{35}. Since then, scars have been observed in both microwave and optical cavities\textsuperscript{29,30,9,19}. Scarring has also been observed numerically in many systems, including relativistic quantum scars in graphene\textsuperscript{14} and in spin-orbit-coupled atomic gases\textsuperscript{18}.

As we make smaller and smaller devices, it is vital that we achieve a good understanding of the behavior not only of the eigenspectra of particles in confining potentials, but also the structure of the wavefunctions of such particles. Furthermore, devices are bound to have imperfections or impurities. It is therefore also crucially important that we understand how randomly placed impurities will affect the behavior of classical or quantum particles, and even how to use these imperfections to our advantage.

Scientists are beginning to find technological applications for the scarring phenomenon. One such application has been in the creation of two-dimensional microcavity lasers that produce a highly directional beam. In particular, Shinohara \textit{et al.} used the two-dimensional stadium billiard, a fully chaotic system, to work toward such a laser with high-\textit{Q} modes\textsuperscript{28}.

On the other hand, scientists have also needed to avoid scars in chaotic cavities used to produce lasers optimized for imaging\textsuperscript{25}.

If quantum computers are going to become ubiquitous, it will be necessary to find a way to fabricate lasers on chips for interfacing optical information processing and transmission with semiconductor devices for future classical and quantum computing devices. Especially with the type of scarring we describe here, particular directions
can be selected that allow better transmission of wave amplitude in particular directions. In our case, this could be done by creating an “impurity” with a gate, which could turn a scar on or off.

1.1 Traditional scar theory

This section would be incomplete without a short review of traditional scar theory, developed by Eric Heller in the 1980s. It was originally conjectured by Berry (known as “Berry’s conjecture”, or “Berry’s random wave hypothesis”) that wavefunctions in a classically chaotic system would exhibit uniform fluctuations in amplitude across the entire accessible space; they would follow, in the limit that $\hbar \to 0$, the statistics of a random superposition of plane waves and thus the statistics of random matrix theory\(^2\). This is a perfectly reasonable conjecture, as we know that a classical trajectory in a chaotic region of phase space will eventually cover, uniformly, all accessible regions of phase space. Taking a semiclassical perspective, it makes sense that a wavepacket launched in such a system would uniformly cover the space, leading also to a uniformly distributed eigenfunction.

It was shown by Heller, however, that short, isolated classical orbits have a huge impact on the form of quantum wavefunctions in chaotic systems and contribute major corrections to the random wave approximation\(^{12,17}\).

Heller demonstrated that some of the wave functions exhibit a large enhancement of amplitude around classical isolated periodic orbits in position space; he called these enhancements “scars” of the classical periodic orbits.

Heller explained the existence of these scars using a semiclassical argument that begins with the stability matrix. The deviation between two points initially separated in phase space by an infinitessimal displacement at some time $t$ is given in terms of
Figure 1.2: Autocorrelation of Gaussian wavepacket launched in a quartic potential. The strength of the recurrences decays exponentially with time, and the rate at which this occurs determines the bandwidth of the energy spectrum.

the stability matrix $M$, as

$$
\begin{pmatrix}
\delta p_t \\
\delta x_t
\end{pmatrix} = M \begin{pmatrix}
\delta p_0 \\
\delta x_0
\end{pmatrix}.
$$

(1.1)

The stability matrix can be used to propagate a Gaussian wave packet, given by

$$
\psi_G(x, t) = \exp\{i/\hbar[(x - x_t) \cdot A_t \cdot (x - x_t) + p_t \cdot (x - x_t) + \gamma_t]\}\}
$$

(1.2)
where

\[ A_t = \frac{1}{2} \delta p_t \cdot (\delta x_t)^{-1} \]  \hspace{1cm} (1.3)
\[ \gamma_t = \phi_t + \frac{1}{2} \hbar \text{Tr} [\ln (\delta x)^{-1}] \]  \hspace{1cm} (1.4)
\[ \phi_t = \int p_t \cdot dx_t - Et \]  \hspace{1cm} (1.5)

where \( \phi_t \) is the classical action.

Heller began by considering a Gaussian wavepacket, centered at time \( t = 0 \) on the classical periodic orbit, launched along a periodic orbit. The overlap of the Gaussian wavepacket with itself at later times, the autocorrelation function \( \langle \psi_G(0)|\psi_G(t) \rangle \), will
exhibit recurrences at integer multiples of the period of the classical periodic orbit. This is of course a consequence of Ehrenfest’s theorem. As the wavepacket spreads, the autocorreltaion decays to zero as \( \exp\{-n\tau\lambda/2\} \), where \( \lambda \) is the sum over the characteristic exponents of \( M \) and \( n \) represents the \( n \)th recurrence of the wavepacket. Thus, the more stable an isolated periodic orbit, the slower the decay of the quantum wave packet. A sample of such an autocorrelation is shown in Figure 1.2 for a Gaussian wave packet launched in a quartic potential.

A lot of information about the eigenspectrum can be obtained by considering a finite time Fourier transform of the time dependent dynamics, as the behavior of the dynamics at short times has the largest impact on the structure of the spectrum. Later time dynamics only serve to make small changes to the spectrum, a principle that Heller has coined “the sculpting principle”\(^{11}\). The finite time Fourier transform of the autocorrelation function leads to the partially resolved spectrum,

\[
\epsilon_T(\omega) = \frac{1}{2\pi} \int_{-T}^{T} \exp\{i\omega t\} \langle \psi_G | \psi_G(t) \rangle dt. \tag{1.6}
\]

Figure 1.3 illustrates the success of the finite time Fourier transform, where the Fourier transform of the autocorrelation function in Figure 1.2 is taken after the first, second, and third recurrences of the wavepacket launched in the quartic oscillator. By the second recurrence, the overall structure of the spectrum has already been solidly established.

The spacing in time between recurrences gives, under the Fourier transform, a measure of the spacing between bands of states in the eigenspectrum. The bandwidth, proportional to \( \hbar\lambda \), is related to the exponential decay of the recurrences of the autocorrelation function. The Fourier transform of the autocorrelation function for a
Gaussian wavepacket launched in a quartic oscillator is shown in Figure 1.3.

The existence of bands means that the semiclassical wave packet must be concentrated on a smaller number of states. The relevant measure here is the ratio of the bandwidth to the bandspacing,

$$\frac{\lambda}{\omega}.$$  

This is the ratio of the number of states the wavepacket lives on to the number of states one would expect from the work of Berry and Voros$^3$, and tells us whether or not we will be able to resolve individual bands in the eigenspectrum.

Especially if the amplitude is not distributed evenly over states, this implies the existence of eigenstates that have a large overlap with the wavepacket. If $\omega/\lambda \gg 1$, then the wave packet stays localized on the orbit. Since the overlap of the wavepacket with the eigenstate must be constant with time, if the eigenstate in question had large initial overlap with the wavepacket, then it must have large overlap later and so it will have large amplitude everywhere along the periodic orbit.

This shows that there must exist states with enhanced probability along a periodic orbit in phase space. This implies, of course, that there must also be enhanced probability along the periodic orbit in position space, and hence, we have scarring.

It is important to note that an enhancement in the wavefunction due to an island in phase space or due to an integrable portion of phase space with area greater than $\hbar$ is not considered to be a scar, since even a classical wavepacket launched in this region will maintain finite recurrences even as $t$ goes to infinity. The effect of scarring depends upon the existence of stable and unstable manifolds, which do exist around an isolated periodic orbit but do not exist around an island.
1.2 NEW SCARS

The new scars were first observed in a quintic potential scattered with random, Gaussian impurities, that break the symmetry of the system. The impurities are small in width, but larger than a wavelength, so diffraction is not a dominating feature. The strength of the impurities is small compared to the energy. The unperturbed system has circularly symmetric eigenstates with two good quantum numbers.

Here, we will consider the system described above, but it should be noted that other systems have been checked for similar behavior, and the phenomenon is very general. It is present for many types of clean systems including both homogeneous and non-homogeneous functions of $r$. It is also not necessary for the underlying function to be circularly symmetric. In fact, we will consider asymmetric systems presently. Scars are also not unique to the structure of the impurities; they have been seen for impurities of various sizes and strengths.

Traditional scars are created by a single short periodic orbit with corresponding stable and unstable manifolds that cover an area in phase space large enough compared to $\hbar$ to create persistent recurrences. Numerically exploring the phase space of the quintic potential on a scale much smaller than $\hbar$ has not revealed any regions of stable and unstable manifolds that could create a scar via the traditional means. There is also no large underlying island in phase space.

1.3 SINGLE IMPURITY $r^5$ CASE

Let’s begin by considering the simplest case: the circularly symmetric, single impurity $r^5$ potential. We will show that in this case, a scar will be formed and it will “pin” to the impurity.
Without loss of generality, we center the impurity at $\phi = 0$ and at a fixed radius, $r_0$. The circularly symmetric basis states of the clean $r^5$ oscillator come in doublets of degenerate states, which we can think of as the left and right circulating states. These are denoted by

$$
\psi_{r,m}(\rho, \phi) = R_{r,m}(\rho)e^{im\phi}
$$

and a doublet consists of the pair of states $\psi_{r,m}$ and $\psi_{r,-m}$. The states can be written as

$$
\psi_{r,m} = R(r)e^{im\phi}
$$

(1.8)

$$
\psi_{r,-m} = R(r)e^{-im\phi}.
$$

(1.9)

Now we’ll apply perturbation theory by starting with the degenerate pairs. We diagonalize the perturbation projected onto the two dimensional subspace formed by the degenerate states, which gives the perturbation matrix

$$
V_{r,\pm m} = \begin{pmatrix}
\langle \psi_{r,m}|V|\psi_{r,m}\rangle & \langle \psi_{r,m}|V|\psi_{r,-m}\rangle \\
\langle \psi_{r,-m}|V|\psi_{r,m}\rangle & \langle \psi_{r,-m}|V|\psi_{r,-m}\rangle
\end{pmatrix}.
$$

(1.10)

Diagonalizing this gives the first order states which can then be coupled to the other doublets via ordinary non-degenerate perturbation theory. We denote these states $\psi_+$ and $\psi_-$. 

The eigenvectors of a nontrivial, non-singular, Hermitian, $2 \times 2$ matrix are the unique pair of orthogonal states that satisfy $\langle \psi_{\pm}|V|\psi_{\mp}\rangle = 0$. States $\psi_+ \propto \cos \phi$ and $\psi_- \propto \sin \phi$ satisfy these requirements, and therefore must be the eigenvectors of the
perturbation matrix above.

These states can be written in terms of the original basis as

\[ \psi_+ = \frac{1}{\sqrt{2}} (\psi_{r,m} + \psi_{r,-m}) \]

and

\[ \psi_- = \frac{1}{\sqrt{2}} (\psi_{r,m} - \psi_{r,-m}) \, . \]

ie \( \psi_+ \propto \cos \phi \) and \( \psi_- \propto \sin \phi \). In other words, one state is symmetric around the impurity at \( \phi = 0 \) and the other is antisymmetric.

When these states couple to the other doublets, symmetric states will only couple to symmetric states, and antisymmetric states will only couple to antisymmetric states. A sum of such states will lead to a large amplitude centered on the impurity.

1.4 The degenerate harmonic oscillator with random Gaussian perturbations

Before tackling the more complicated quintic potential, which, save for doublets, has no exact degeneracy, let’s consider a system with perfect degeneracy. A natural choice is the classical two-dimensional 2:1 harmonic oscillator, which has a frequency in one direction that is twice the frequency in the orthogonal direction. The clean 2:1 harmonic oscillator contains four types of classical periodic orbits which are reflected clearly in the quantum states shown in Figure 1.4. The trivial, shortest orbit is the “bouncing ball” orbit that oscillates back and forth through the center of the well in either direction; this can be seen in the upper left tile in Figure 1.4. There also exists a “figure-eight” orbit, which, as its name suggests, traces a figure-eight. Finally,
there are orbits that lie between figure-eight and banana, which look like a squished figure-eight or a banana.

Figure 1.5 shows the composition of the eigenstates of the full Hamiltonian as a sum of the basis states of the clean 2:1 oscillator. The basis states of the clean oscillator are shown along the vertical axis and are ordered by increasing action in one dimension (and decreasing action in the other direction). Red tiles represent a large negative contribution and blue tiles represent a large positive contribution, while white represents no contribution. Each state of the full Hamiltonian is composed of basis states that are close in action. This demonstrates that the perturbation mixes unperturbed states with similar actions.

If you watch the evolution of a periodic trajectory in the clean system, the trajectory will simply retrace itself for all time. If the perturbation is turned on, the trajectories will of course in general no longer follow the periodic trajectory of the clean system. However, as long as the perturbation isn’t enormous, a trajectory will still spend a lot of time in orbits that are similar to the periodic orbits of the clean system. Trajectories actually move from nearly figure-eight to nearly banana, transitioning between them in an orbit that is the “superposition” of the two. The crucial thing is that the trajectories spend a lot of time in almost-periodic motion, even when the perturbation is not miniscule.

In these cases there are not islands in phase space, but, rather, “sticky” regions around what were once purely islands, where chaotic orbits will linger for a while before getting kicked off into the depths of the chaotic sea. The possibility that such sticky regions play a role in the scarring of the quintic potential is worth exploring. It may be possible to make a semi-classical argument that gives the same result as the perturbative argument.
Figure 1.4: Eigenstates of the degenerate 2:1 oscillator with random perturbation. The lower middle and lower right states are nearly figure-eight states, with a touch of banana, and there are about 4 states exhibiting banana motion. The upper left hand state is a bouncing ball.
Figure 1.5: Composition of perturbed states in terms of clean oscillator eigenstates. Perturbed states (along the horizontal axis) shown as a sum of unperturbed basis states (along the vertical axis) in the degenerate harmonic oscillator. The redder the square the more negative the contribution from the basis state, while the bluer the square the more positive the contribution from the corresponding basis state. The figure demonstrates that the coupling due to the perturbation is local in action space.
There is a time scale, called the “log time” or the “break time,” which can be understood to be the timescale it takes for classical dynamics to develop fine structure - less than area $h$ in phase space. If a cluster of trajectories remain in a region less than $h$ in the Poincare surface of section, and do not leave this area within the characteristic break time, this could lead to a quantum enhancement. The quantum mechanics can only resolve areas in phase space on the order of $h$, and anything smaller than this cannot be resolved. In other words, quantum mechanics may not be able to distinguish between an exactly periodic orbit and a nearly periodic orbit.

Another way to look at this is that the quantum spectrum is the Fourier transform of the autocorrelation function. If a quantum wavepacket is launched along a nearly periodic orbit within a sticky region, the overlap upon its return to its initial location will be nearly the same as that of the case of an exact periodic orbit- the same argument used in traditional scar theory. Because there is a finite time in which the gross features of the eigenvalue spectrum can be resolved, the quantum mechanics won’t care if the wave function drifts away at longer times, as long as it hangs out around the periodic orbit long enough for the quantum mechanics to be established.

To emphasize that this is not specific to the 2:1 harmonic oscillator, another example of quantum states resembling classical trajectories is shown in Figure 1.6. This figure shows a state of the 1:1 harmonic oscillator, whose classical periodic orbits are elliptical. The state shown can be thought of as a superposition of two classical elliptical orbits.

1.5 The $r^5$ Oscillator

Let’s begin by considering the clean, circularly symmetric classical quintic oscillator. In this system, the shortest periodic orbit is the trivial “bouncing-ball” orbit, which
is just an orbit that traces out the same line back and forth across the oscillator; in other words, it doesn’t circle around the origin. A small deviation from this launch angle will cause the particle to rotate in the angular direction as it oscillates in the radial direction. When the particle is launched so that the frequencies of the radial and angular directions match the resonance in the system, the trajectory follows a periodic orbit.

The smallest nontrivial periodic orbit in the quintic potential comes from the 5:2 resonance, which manifests itself in general as a star in position space; the particle oscillates five times in the radial direction in the time it takes to cycle the center twice. This system also contains other periodic orbits, like the seven and nine pointed stars, but these periodic orbits are longer and have less of an influence on scarring.

Each quantum state in the clean quintic oscillator has rotational symmetry and therefore has an exactly degenerate partner. One can think of this pair of states as
Figure 1.7: Energy as a function of radial quantum number, with the angular quantum number decreasing as \( r \) increases. The blue data is a resonant set achieved by exchanging two quanta in the radial direction for five quanta in the angular direction: a 2:5 resonant set. The green data represents a 3:7 resonant set.

left and right circulating states. Other than the pairs within each of these doublets, all doublets have a unique energy specified by the radial quantum number \( r \) and the absolute value of the angular quantum number \( m \).

Unlike the case of the harmonic oscillator, the energy levels are not spaced evenly in the quintic oscillator. The Bohr correspondence principle tells us that the spacing is proportional to the frequency which depends on the action,

\[
\Delta E \propto \omega.
\]

(1.11)

In the classical system, a periodic orbit exists precisely when the oscillation frequencies of two or more actions are commensurable. For example, in the \( r^5 \) oscillator there exists a 2:5 resonance between the angular and radial actions. The direct consequence
of this is that a particle will oscillate five times in the radial direction in the time it takes to orbit the center twice in the angular direction. Classically, this produces a star-shaped periodic orbit. Therefore, if a quantum state is close in action to this classical periodic orbit representing a 2:5 resonance, then the change in energy from shifting five quanta in radial momentum will be very close to shifting two quanta in angular momentum, although not exact. Therefore, an exchange of two quanta of radial momenta for five quanta of angular momenta will yeild a state that is close in action and close in energy.

For a set of resonant states, defined as the set of states achieved by trading two units of angular momenta for five units of radial momenta, there will exist a point along this set that is near the classical orbit; that is, the ratio of the frequencies in the radial and angular directions will be five to two. Figure 1.7 shows the energies of the states in a resonant set for both the 2:5 resonance and the 3:7 resonance. Near the top of the peak in this plot, the energies of adjacent states are very similar. While there may be other states within this energy range, those states will be a part of other resonant sets and will thus be far away in action. The spatial overlap of the two wavefunctions will therefore be small, and the states will not couple strongly even though the difference in energy between the states will be small. Nearness in energy and similarity in wavefunction are both needed for a strong overlap between two states.

1.5.1 Perturbation theory on the quintic potential

Now that we understand the structure of the eigenstates and the underlying resonances of the quintic potential, we’re ready to add a perturbation. The perturbation will consist of randomly scattered Gaussian impurities. Although similar behaviour is observed for other types of impurities, we will use Gaussians without loss of general-
ity. We start with the time independent potential,

\[ H = H_0 + \lambda V \]  \hspace{1cm} (1.12)

where

\[ H_0 = \frac{\hbar^2}{2\mu} \nabla^2 + r^5 \]  \hspace{1cm} (1.13)

and \( V \) is the perturbation. The width of the impurities is greater than the wavelength of the states, meaning that diffraction is not the dominant effect, and the strength of the impurities is small compared to the energy of the wave. The spacing between the bumps is on par with or greater than the characteristic size of the impurities themselves, although this was not found to have a substantial effect on the results numerically.

How does this perturbing potential couple the states of the clean oscillator that we discussed in the previous section? The nature of the perturbing potential is such that the perturbation induced coupling will be local in action space. This can be seen by examining the overlap between just the angular part of the wavefunction of two states with actions that differ by \( a \) quanta:

\[ \langle \psi_m | V | \psi_{m+a} \rangle = \int e^{-im\phi} V e^{i(m+a)\phi} d\phi \]  \hspace{1cm} (1.14)

\[ = \int e^{ia\phi} V d\phi. \]  \hspace{1cm} (1.15)

This is the Fourier transform of \( V \), and as \( a \) increases, this integral will fall off rapidly as the exponential oscillates more and more rapidly. The radial part behaves similarly, and the locality of the coupling matrix can be seen in Figure 1.8; the matrix elements are larger along the diagonal. This means that the coupling is local in action
Figure 1.8: The coupling matrix, $\langle \psi_i | V | \psi_j \rangle$, displayed on the left. The data on the right hand side is the same as the matrix on the left with the data clipped to show the fine structure of the off-diagonal matrix elements.

This means that when a small perturbation is applied, the resulting states will be composed mostly of these states that are similar both in energy and in action. With this in mind, it is appropriate to treat the set of quasi-degenerate states around the peak of the curve in Figure 1.7 with degenerate perturbation theory, as long as we only apply it on the quasi-degenerate manifold.

In the clean system, every state has a degenerate partner which we can think of as left and right circulating states. The introduction of the perturbation breaks this degeneracy, leaving us with a truly non-degenerate set of states.

If we treat the few states at the top of the resonant set curves shown in Figure 1.7 as a degenerate subspace- an approximation that gets better and better with increasing energy- a beautiful thing happens. In the degenerate case, the perturbed energies
and eigenstates are given by the eigenvalues and eigenvectors of the coupling matrix

\[ W = \langle \psi_0 | V | \psi_0 \rangle. \] (1.16)

where \( |\psi_0\rangle \) are the eigenstates of the clean system. This will result in a set of perturbed, non-degenerate set of eigenstates of \( V \) which we’ll denote as

\[ |\phi_i\rangle. \]

Because the states are now non-degenerate, one of them will have a maximum eigenvalue and one will have a minimum such that

\[ W|\phi_1\rangle = \epsilon_1|\phi_1\rangle \] (1.17)
\[ W|\phi_2\rangle = \epsilon_2|\phi_2\rangle \] (1.18)
\[ \vdots \] (1.19)
\[ W|\phi_n\rangle = \epsilon_n|\phi_n\rangle. \] (1.20)

where we’ll define the states such that \( \epsilon_1 > \epsilon_2 > \ldots > \epsilon_n \). By definition, the resulting eigenstate with the highest or lowest eigenvalue is the state that maximizes or minimizes the overlap with the perturbation, which we will now prove.

Consider an arbitrary state expressed in the above eigenbasis,

\[ |\psi\rangle = \sum_i a_i|\phi_i\rangle \]

where \( \sum_i |a_i|^2 = 1 \).

The overlap with the perturbation is given by.
\[ \langle \psi | W | \psi \rangle = \sum_i \sum_j \langle \phi_j | a_i a_j^\dagger W | \phi_i \rangle \]  \hspace{1cm} (1.21)

\[ = \sum_i \sum_j a_i a_j^\dagger \langle \phi_j | W | \phi_i \rangle \]  \hspace{1cm} (1.22)

\[ = \sum_i \sum_j a_i a_j^\dagger \langle \phi_j | \epsilon_i | \phi_i \rangle \]  \hspace{1cm} (1.23)

\[ = \sum_i \sum_j a_i a_j^\dagger \epsilon_i \langle \phi_j | \phi_i \rangle \]  \hspace{1cm} (1.24)

which is only non-zero when \( i = j \). This gives

\[ \langle \psi | W | \psi \rangle = \sum_i |a_i|^2 \epsilon_i. \]  \hspace{1cm} (1.25)

What combination of the states \( |\phi_i\rangle \) produces the largest overlap with the perturbation? Since Equation 1.25 is simply a weighted average, the overlap \( \langle \psi | W | \psi \rangle \) is maximized for the state \( |\psi\rangle \) that is composed of the single \( |\phi_{\text{max}}\rangle \) with the largest eigenvalue \( \epsilon_{\text{max}} \). The sum is maximized for the largest value of epsilon when all the other a\( s \) are zero. There can be no other combination of the initial states, \( |\phi_i\rangle \), that can increase the overlap with the perturbing potential, as adding any other state will reduce the value of the weighted average.

Crucially, the maximization and minimization predicts a unique orientation of the scar, since in general, for a random distribution of impurities, there will only be one orientation that extremizes the overlap.

Degenerate perturbation theory also tells us that the eigenstate with the highest eigenvalue and the eigenstate with the lowest eigenvalue must in general be the most scarred states in the set. This is because, for a randomly generated potential \( V \), a
state that is non-local will simply give an average of the potential. In order for a state
to have maximum overlap with a random potential, it therefore must be localized.

Of course, there will be small corrections to the orientations when all the states
are considered. These corrections, however, will be much smaller than the dominant
effects from the pseudo-degenerate manifold.

This argument can be viewed as a variational principle.

1.6 PERFORMANCE OF DEGENERATE PERTURBATION THEORY

To demonstrate the effectiveness of this argument, we have plotted the predictions of
degenerate perturbation theory in Figure 1.9 with the same states calculated exactly
in Figure 1.10. The perturbing potential is shown in Figure 1.11.

Degenerate pertubation theory on the pseudo-degenerate manifold of states in the
resonant set gets the general features of the stars and correctly reproduces their orient-
tations. Fine close agreement is pictured in Figure 1.12, where a single contour of the
state calculated using perturbation theory is plotted over the wavefunction calculated
with itp2d.

1.6.1 OFF-RESONANT HARMONIC OSCILLATOR

Finally, we briefly considered fully non-degenerate harmonic oscillators and propose
that future work be done to completely understand the mechanism behind the for-
mation of eigenstates in this case. These are those oscillators that have irrational fre-
quency ratios of, say, 1 : π, with a perturbing impurity potential. Considering such
off-resonant harmonic oscillators is important because in systems like these, there are
no short underlying periodic orbits. The classical orbits of such a system will still be
Figure 1.9: States calculated via degenerate perturbation theory on a small subset of states within a resonant set.
Figure 1.10: States calculated (almost) exactly via diagonalization on a very large subset of basis states.
Figure 1.11: The perturbing potentials responsible for the states shown in Figures 1.9 and 1.10.

Lissajous curves; they will, however, be quasiperiodic, filling a two-dimensional area in phase space.

One might expect that in this case, the eigenfunctions would simply be more spread out, covering the same spatial area covered by the quasiperiodic Lissajous curve. This is not, however, what we see.

The eigenfunctions of such Hamiltonians did not represent such quasiperiodic trajectories, but, rather, displayed periodic orbits of nearby degenerate systems, such as the 2:1 oscillator. The figure-eight orbit, the bouncing ball orbit, and the banana orbit were all still present, and are shown in Figure 1.13. The potential used to generate these results was a nearly 2:1 oscillator with a random scattering of impurities, and the eigenfunctions are clearly showing states characteristic of the 2:1 oscillator, which is nearby in some sense. Scarring by a single impurity is shown in Figure 1.14.

I propose that the explanation for such a phenomenon is that these trajectories are encountering sticky regions such as those discussed previously in this chapter.
Figure 1.12: Results of degenerate perturbation theory overlayed on results from `tp2d`. The data from `tp2d` was kindly supplied by P.J.J. Luukko. A single contour of the eigenstate from perturbation theory is displayed. The agreement between the exact eigenstate and the state formed using only a few eigenstates of the clean system is exquisite.
Figure 1.13: Eigenstates of a the non-degenerate harmonic oscillator, approximately 2:1, which has no underlying classical figure-eight or banana trajectories. The states shown closely resemble the states one would expect for the exact 2:1 harmonic oscillator.
Figure 1.14: An example of a state formed with a single impurity in the non-degenerate harmonic oscillator.

1.7 Conclusion

In summary, there are two important ingredients that contribute to the formation of this new type of scar. The first is that the underlying classical resonance implies that the states resulting from the perturbation will be a sum of states related by the 5:2 resonance. This means that the resulting eigenstates of the perturbed system can range from a “donut”, the most delocalized state, to a “star,” the most localized state that can be made from this sum. Because perturbation theory tells us that the one of the perturbed eigenstates will be the state that maximizes the overlap with the potential, and another of the perturbed eigenstates will minimize the overlap with the potential, a state that maximizes or minimizes overlap with a random potential must be localized in position space in order to extremize the overlap. Otherwise, if the state was evenly distributed over the potential, the state overlapped with the po-
tential would simply be an average of the potential, not an extremum.

This scarring phenomenon could have many applications and implications in many areas. It’s nearly impossible, for example, to get perfectly clean experimental systems; there is almost always some impurity potential marring a microscopic cavity. One should be able to control wave functions within such a cavity by introducing a new component of the potential. The wave function in the cavity would then change in order to maximize the overlap, and in this way control the geometry of the wave function.

It could be very useful in experiments, as all it would take to pin down a wavefunction is a single perturbation to the potential.
2

The kick and drift model

2.1 Introduction

Flows traversing smoothly disordered potentials exhibit branching, where the current splits off into several relatively strong streams. This was not obvious, and it was a surprise to the Westervelt group who observed this phenomenon in electron waves traversing a two-dimensional electron gas in the early 2000s. Their experiment spurred a wave of research into this phenomenon of branched flow, and the classical formation of caustics was implicated as the root cause of the phenomenon.

Branched flow is a ubiquitous phenomenon occurring whenever a collection of particles or waves traverses a weak, smooth, correlated random potential. It has been
found that the intensity distribution of such flow has a heavy tail, meaning extremely high density occurs with greater frequency than would be predicted by random wave models\textsuperscript{37,34}. This phenomenon is present in both quantum and classical flows, through random potentials displaying a broad range of correlation functions, so long as the correlation length of the potential is longer than the characteristic wavelength of the flow. It has been observed or predicted in systems with length scales spanning at least twenty orders of magnitude, from two-dimensional electron gases\textsuperscript{31}, to radio waves propagating through the interstellar medium\textsuperscript{8,26}. Branched flow is also believed to influence the propagation of tsunamis and the appearance of freak waves in the ocean\textsuperscript{37,13}.

The strong fluctuations in the intensity of waves propagating through weakly random media have been extensively studied, particularly in the far field regime, but a detailed understanding of the early behavior of such flows - during the first few generations of caustic formation, in which the most extreme fluctuations occur - is lacking. The presence of a caustic is a necessary but not sufficient condition for the presence of a strong branch; the intensity of the branch corresponding to a caustic is governed by the stretching or compression of the classical phase space along the direction of the manifold of trajectories. To illuminate this regime, we introduce a simple model which captures the key features of such branched flow. We show here that caustic formation and manifold compression go hand in hand. Under the influence of a random potential, a manifold in phase space will develop intricate structure, stretching and folding over on itself. The strength of the flow in position space is found by projecting this convoluted manifold onto the spatial coordinates – a radon transformation (see Figure 2.1). Hence, at caustics, where the slope of the manifold $dp/dx$ is infinite, the density of the flow formally diverges. We note that in real physical systems, there is
Figure 2.1: A manifold of trajectories in phase space that have undergone propagation via the kick and drift model. The dot density (upper panel) shows the variation in the stretching of the manifold, and the projection onto phase space (lower panel) shows the density in position space. Qualitatively, the kick and drift map shows the same features displayed by quasi-two-dimensional dynamics or full two dimensional dynamics.

always an effective spatial averaging on some length scale determined, for instance, by the characteristic wavelength of the system or the uncertainty principle. This serves to smooth over the divergences and keep the flux finite even where the slope of the manifold is infinite. These folds, known as caustics, are the origin of branches\textsuperscript{16}. A simple caustic is shown in Figure 2.2.

However, not all caustics lead to intense branches. Many caustics, especially in the far field region of the flow, do not carry sufficient flux to stand out above the average background flow rate; this happens when a branch forms in a region where the manifold has been stretched considerably. Also, some caustics are in parts of the manifold which exhibit strong curvature and therefore do not translate to a strong branch after a radon transformation. Thus, the presence of a caustic is a necessary but not suffi-
Figure 2.2: A line of trajectories, uniformly distributed along the x axis is launched with momentum in the y direction. As the trajectories reach the dip in the potential, they acquire momenta in the x direction. The phase space diagram at the slices shown on the left are plotted on the right hand side.
cient condition for the presence of a substantial branch.

Previous work by Kaplan\textsuperscript{16} incorporates both the stretching of the trajectory manifold and the rate of formation of caustics to provide expressions for the number and intensity of strong branches in the far field regime, while the work of Metzger et al.\textsuperscript{23} provides a formula for the number of caustics, applicable even in the near field regime and the distribution of strong branch intensities\textsuperscript{24}. However, a detailed understanding of the influence of trajectory manifold stretching on the early, strong branching regime is lacking.

Unlike prior studies, we show that increased density along a trajectory manifold is intimately tied to the formation of caustics. In fact, caustic formation always locally increases the density of particles along a manifold, meaning that there are three factors contributing to the intensity of branches: manifold divergence, compression, and curvature around caustics.

2.2 A SINGLE CAUSTIC

A natural place to start to gain intuition for the effect of a smooth potential is to look at the effect of a single valley on a uniform flow. Figure 2.2 shows the formation of a caustic due to a single feature- a Gaussian valley - in the potential. A plane wave front in the form of a manifold of trajectories is propagated over the potential, and the manifold is plotted in phase space on the right. It is initially horizontal, as the entire wavefront has the same momentum, but it is evenly spread in position.

As the wavefront propagates over the depression in the potential, the particles on the right experience a force to the left, and the particles on the left experience a force to the right. This decreases and increases the momentum of the particles, respectively, and the manifold is pinched and twisted as the trajectories form a caus-
Figure 2.3: The evolution of a manifold of trajectories under propagation with the kick and drift map. The dot density shows the evolution of the stretching of the manifold over time, in a way that can’t be seen with a simple line with zero thickness.

tic. In phase space, the slope in the center of the manifold becomes infinite, and two cusps (also with infinite slopes) propagate away. The phase space picture is somewhat deceptive, however, and becomes more enlightening if we consider discretely placed particles rather than a line. Figure 2.3 shows the phase space evolution of initially uniformly spaced points in phase space under the “kick and drift map,” which we will discuss shortly. The qualitative nature of the evolution of the map is the same as that of particles traversing a smooth potential with randomly spaced potential bumps.
2.3 The Kick and Drift Model

Consider a manifold of initial conditions in phase space, uniformly distributed in position and all with the same momentum—this is a line parallel to the position axis, just like what we considered in the previous section. As they propagate, they encounter a position dependent potential. If the potential is weak compared to the energy of the particles, the force from the potential will induce a weak, position dependent shift in the momentum of the flow. Since the change in momentum is small, there is little displacement of position during the time that the flow takes to traverse the region occupied by the potential feature; significant displacements only develop after the flow has left the region where the change in momentum occurred. Thus, the effect of a small bump or dip in the potential resembles that of a discrete kick that changes the momentum instantaneously. Furthermore, to first order in the strength of the random potential, the distance travelled in the initial direction of propagation will be proportional to time\(^{16}\). With this in mind, we propose a discrete map which mimics the behavior of the full two-dimensional system but provides a simpler framework for numerical and analytical study.

The map, which we will call the “kick and drift” map, is defined as

\[
p_{n+1} = p_n - \frac{dV_n(x)}{dx} \tag{2.1}
\]

\[
x_{n+1} = x_n + p_{n+1} \tag{2.2}
\]

where \(p\) and \(x\) are analogous to the transverse position and transverse momentum in the two-dimensional problem. This is a generalization of the standard map, where the “kick” term, \(V_n(x)\), is a smooth, random potential correlated in \(x\) and independent
of all previous and future kicks, instead of a sinusoid. This Hamiltonian map can be interpreted physically as free particle propagation in one dimension interrupted by the application of instantaneous kicks at regular intervals.

Although branched flow can appear in potentials displaying a broad range of smooth correlation functions\textsuperscript{23}, we will follow previous authors in taking a Gaussian correlated potential\textsuperscript{16,36} such that

$$V_n(x) = 0, \quad V_n(x)V_n(x') = v_0^2 e^{-|x-x'|^2/\xi^2}. \quad (2.3)$$

The flow pattern from such a map displays behavior strikingly similar to the full two-dimensional model, developing the same intricate convolutions in phase space and the same dependence of time to the onset of caustic formation on potential strength, $t_c \propto v_0^{-2/3}$, as the full two dimensional system. (Note that the sequence of kicks in the figure is not meant to mimic the full two dimensional system– when we say they are similar we mean the average features are the same.) The trajectory density for the full two-dimensional potential is shown in Figure 2.4, and the trajectory density for the map is shown in Figure 2.5. Note that the qualitative behavior is indistinguishable.

Now that we have established that the more tractable “kick and drift” map picture captures all the necessary elements for producing branched flow, we will take a close look at the evolution of the map in its two-dimensional phase space, starting with the slope of the manifold.
Figure 2.4: Trajectory density from trajectories launched over a full two dimensional potential.

Figure 2.5: Trajectory density from a simulation of 3000 iterations of the kick and drift map.
2.4 The effect of phase space dynamics on manifold slope

To understand the relationship between manifold density and caustics we must examine the mechanism by which caustics form. A caustic is defined to be a point where the derivative $\frac{\partial p}{\partial x}$ along the trajectory manifold is infinite. Because the potential and its first derivative are finite, the “kick” step will cause a finite change in the slope of the manifold. It is therefore only the uniform shearing of phase space during a drift step that creates formal divergences in $\frac{\partial p}{\partial x}$.

In the weak kick regime individual kicks cause only small changes in the slope $\frac{\partial p}{\partial x}$ of the manifold; caustics begin to form only after many iterations of the map have transpired. Note that we are interested only in caustics which develop as a result of interactions with the potential; we are not concerned with caustics which might form due to the initial conditions of the system even in the absence of a random potential. A kick changes the slope of the trajectory manifold at a point $a$ by

$$\left.\frac{\partial p}{\partial x}\right|_a \rightarrow \left.\frac{\partial p}{\partial x}\right|_a - \left.\frac{\partial^2 V}{\partial x^2}\right|_a$$

while a drift step will change the same slope by

$$\left.\frac{\partial p}{\partial x}\right|_a \rightarrow \left(1 + \left.\frac{\partial p}{\partial x}\right|_a\right)^{-1} \left.\frac{\partial p}{\partial x}\right|_a$$.

Note that the change in slope effected by a kick does not depend on the current slope of the manifold, while the change effected by a drift does. Crucially, the change in slope due to a single drift step diverges for segments of the trajectory manifold with initial slope $-1$, and it is monotonically increasing on the interval $(-1, 0]$ (see Figure 2.6). Thus, for any random potential whose derivative is bounded, there will
Figure 2.6: The effect of a shear on a variety of sloped line segments. On the top, equal length line segments (yes, they really all have the same length) at various angles. The bottom shows the line segments after a shear has been applied, equivalent to a “drift” step in the kick and drift map. The degree of stretching or compressing varies greatly depending on the initial slope of the manifold.
be a critical slope between $-1$ and $0$ below which the slope must continue to decrease until a caustic forms. In other words, there is a slope at which the the effect of drift steps will dominate the effect of kicks, and a segment of manifold which passes this critical slope will then be drawn inexorably into a caustic. For weak potentials, this critical slope will be very small.

2.5 The effect of phase space dynamics on manifold stretching

We now turn our attention to the mechanism by which the trajectory manifold is stretched or compressed. The kick and drift map is already unit-less, so position and momentum are already on equal footing in this model. The length of an infinitesimal segment of the manifold is therefore given by

$$
\delta s = \sqrt{\delta p^2 + \delta x^2} = \delta p \sqrt{1 + \left( \frac{\partial x}{\partial p} \right)^2} = \delta x \sqrt{1 + \left( \frac{\partial p}{\partial x} \right)^2}.
$$

A drift step leaves $\delta p$ unchanged, while a kick step leaves $\delta x$ fixed.

Therefore, a drift step that increases $\left| \frac{\partial p}{\partial x} \right|$ of the infinitesimal segment or a kick step that decreases $\left| \frac{\partial p}{\partial x} \right|$ compresses the manifold; likewise, the manifold is stretched ($\delta s > 0$) wherever the opposite conditions are met. The length of an infinitesimal segment of the manifold about a point $q$ changes by a factor of

$$
S_{\text{drift}} = \sqrt{\frac{1 + 2 \left| \frac{\partial p}{\partial x} \right|_q + 2 \left| \frac{\partial p}{\partial x} \right|_q^2}{1 + \left| \frac{\partial p}{\partial x} \right|_q^2}}
$$

under the influence of a single drift step. One can readily see that portions of the manifold with small negative slope, $-2 < \frac{\partial p}{\partial x} < 0$, are compressed during a drift step.
For a kick step, the manifold is stretched by a factor of

\[ S_{kick} = \sqrt{\frac{1 + \left| \frac{\partial p}{\partial x} \right|_q + \left| \frac{\partial^2 V_n}{\partial x^2} \right|_q^2 - 2 \left| \frac{\partial p}{\partial x} \right|_q \left| \frac{\partial^2 V_n}{\partial x^2} \right|_q}{1 + \left| \frac{\partial p}{\partial x} \right|_q^2}}. \quad (2.5) \]

We note that this is true for any canonical transformation that preserves the caustics, which in this case is a constant scaling of the position and momentum coordinates. If we make a transformation such that \( \alpha p = p' \) and \( \beta x = x' \), the critical slope occurs at \( \frac{\partial p}{\partial x} = -\frac{\alpha}{\beta} \) and the manifold is compressed when \( 0 < \frac{\partial p}{\partial x} < -\frac{2\alpha}{\beta} \). Note that for the case where \( \alpha = \beta = 1 \) we get the ranges given above.

The kicks are assumed to be uncorrelated with one another, and therefore their effect on the rarefaction can be viewed as a random walk. On the other hand, drift steps have a deterministic effect on the rarefaction, and once the critical slope is exceeded every subsequent drift step will cause compression of the manifold until a caustic is encountered. It follows that the density of trajectories along the manifold will always be elevated at caustics.

Note that this phenomenon, though it can be understood more readily in the kick and drift model, is not unique to this particular model; compression at caustics will occur in any dynamical system in which there is a deterministic linear momentum dependent shearing of phase space along with small, random position dependent deformations. In the case of a flow over a smooth two-dimensional random potential, position and momentum dependent shearing of phase space happen continuously and simultaneously. Nevertheless, so long as the potential is weak enough that the deflections induced by traveling across one correlation length are themselves much smaller than one correlation length, compression will generically occur at all caustics.
2.6 The rarefaction exponent

To quantify the local density of trajectories in phase space we use the rarefaction exponent introduced by Heller and Shaw\textsuperscript{27}:

\[ r(t) = \log |\mathbf{M}(x_0, x_t) \cdot \tilde{d}(x_0)| \]  

(2.6)

where \( \tilde{d}(x_0) \) is the normalized tangent vector to the initial manifold of trajectories at a point \( x_0 \) and \( \mathbf{M}(x_0, x_t) \) is the stability matrix evaluated along the trajectory from \( x_0 \) to \( x_t \). The rarefaction measures the local deformation of phase space along the manifold of trajectories, directly quantifying the density of trajectories. This is an advantage over the stability exponent, which instead approximates the largest eigenvalue of the stability matrix which may correspond to an eigenvector with small overlap with the trajectory manifold. It is important to note that the rarefaction will in general vary widely along the evolving manifold, as can be seen in Figure 2.7, which shows the rarefaction of a manifold of trajectories after 2500 iterations of the kick and drift map, and in Figure 2.3, which shows an example of just the first ten iterations of the map. The definition of rarefaction does require that a norm be specified for phase space. For our purposes, the standard L2 norm with a fixed scaling of phase space suffices.

As you can see in Figure 2.8, the rarefaction increases linearly with time on average. When a trajectory enters the compressive region leading to a caustic, that is, when the manifold around that trajectory passes the critical slope, the rarefaction begins a logarithmic decrease as the trajectory approaches the caustic, although it cannot actually diverge at the caustic because of Liouville’s Theorem.
Figure 2.7: A phase space plot of kick and drift data showing one thousand trajectories after 2500 iterations of the map with a kick strength of $v_0 = 10^{-6}$ and a correlation length of $\xi = 0.1$. The trajectories initially had zero momentum and were uniformly spaced between $x = 0$ and $x = 1$. The color of each point is the rarefaction calculated along the corresponding trajectory. The color and the visible variation in dot density clearly demonstrate the correlation between caustics and manifold compression.

We define the compression at a caustic, $\lambda_c$, to be the difference between the rarefaction at the caustic and the rarefaction at the point immediately before the trajectory began its descent into the caustic, i.e. the previous local maximum. Figure 2.9 shows the distribution of $\lambda_c$ for several different kick strengths, $v_0$. The typical compression factor at caustics displays a dependence on kick strength which is in good agreement with the predicted $\lambda_c \propto v_0^{-2/3}$ scaling law (Figure 2.8).

Figure 2.7 shows how a manifold of trajectories, which was initially uniformly distributed along the line $p(x) = 0$ in phase space, is distorted by the kick and drift map. It is apparent that the degree of stretching of the manifold varies greatly; in this case, after 2500 iterations the trajectory density spans more than four orders of magnitude.

Notice also that caustics are always accompanied by very low rarefaction. Indeed, simulations of both kick and drift and full two-dimensional dynamics demonstrate
Figure 2.8: Rarefaction as a function of time for five typical kick and drift trajectories with different kick strengths, $v_0$. The horizontal axis has been scaled by $t_c$ for each curve so that the typical spacing between caustics is the same. The vertical axis scaling is the same for all curves. The increased compression with decreased kick strength is evident by the depth of the dips at caustics.

Figure 2.9: Probability density functions of the compression at caustics, $\lambda_c$, for five different values of the potential strength, $v_0$, in the kick and drift model.
that compression is always present at caustics.

There are two factors which determine the intensity of the branch caused by a caustic: the density of trajectories along the manifold and the curvature of the manifold at the caustic. Here we derive expressions for the probability distribution of rarefactions at a caustic and the probability distribution of curvatures at a caustic.

First we will determine how many iterations of the map are required to reach the first generation of caustics. We shall accomplish this by deriving a set of stochastic differential equations governing the slope of the trajectory manifold at a point. When this slope diverges, we have reached a caustic.

The behavior of the slope changes dramatically around the critical slope - the slope at which the effect of a drift step is greater than the effect of any kick. In particular, once the critical slope is reached the trajectory will be drawn inexorably into a caustic. Therefore, it is worthwhile to calculate the critical slope in terms of the characteristics of the kick potential (i.e. strength and correlation length).

2.7 Critical Slope

To calculate the critical slope, first recall that the Kick and Drift map is defined by the following,

\[
\begin{align*}
    p_{n+1} &= p_n - \frac{dV_n(x)}{dx} \\
    x_{n+1} &= x_n + p_{n+1}
\end{align*}
\]  

\tag{2.7} \tag{2.8}

where \( p \) and \( x \) are analogous to the transverse position and transverse momentum in the two-dimensional problem. We typically consider a Gaussian correlated random
potential with correlation function

\[ V_n(x)V_n(x') = v_0^2 e^{-|x-x'|^2/\xi^2} \]  

(2.9)

The second derivative of such a potential with respect to \( x \) will be on the order of \( \frac{v_0^2}{\xi^2} \). For notational convenience we will define a quantity \( c_0 \equiv \frac{v_0}{\xi^2} \).

By considering the effect of one iteration of the map on two points initially separated by an infinitesimal displacement in phase space, one can readily derive that the local change in the slope of a trajectory manifold is

\[ \Delta m = \frac{mV'' - m^2 - V''}{1 + m - V''} \]  

(2.10)

where \( m \equiv \frac{\partial p}{\partial x} \) and \( V'' \equiv \frac{\partial^2 V}{\partial x^2} \). We wish to find the critical slope, \( m_c \), which will be the slope at which equation (2.10) is negative for any kick, hence also for the maximum magnitude of \( V'' \). Substituting \( -c_0 \) for \( V'' \) will give us the correct order of magnitude. Doing so yields

\[ m_c = -c_0 - \frac{\sqrt{c_0^2 + 4c_0}}{2} \]  

(2.11)

Recall that we are interested in the regime where the potential is very weak. We can therefore approximate the critical slope by the leading order term in \( c_0 \), which yields simply

\[ m_c = -c_0^{1/2}. \]  

(2.12)

2.8 Evolution of the slope

Now we wish to understand in a probabilistic way how the slope changes as the map iterates. We wish to simplify equation (2.10) in the limit that \( V'' \) and \( m \) are small,
but allowing the two small quantities to vary relative to one another. Using only the $V''$, $m << 1$ limit, we can rewrite (2.10) as

$$\Delta m = (mV'' - m^2 - V'')(1 - m + V'')$$

(2.13)

Now we can consider various regimes: In the regime where $m << m_c$ we will typically have $m^2 << V''$, so (2.13) becomes

$$\Delta m = -V''$$

(2.14)

When $m m_c$ we have $m^2 V''$, so

$$\Delta m = -m^2 - V''$$

(2.15)

When $m >> m_c$ we have $m^2 >> V''$, so

$$\Delta m = -m^2$$

(2.16)

We see that for slopes small compared to the critical slope the slope effectively executes a simple random walk, for slopes large compared to $m_c$ the slope behaves like $m_n \propto (n - n_0)^{-1}$ for some $n_0$, while for the regime near the critical slope we have some more complicated behavior wherein a deterministic drift is accompanied by random jitters of comparable magnitude.
2.9 Rarefaction

The ratio of the length of an infinitesimal segment before and after a single iteration of the map gives

\[
\frac{L_{n+1}}{L_n} = \sqrt{2} \left( \frac{(\Delta V' - \frac{1}{2} dx - dp)^2 + \frac{1}{2} dx^2}{dx^2 + dp^2} \right)^{\frac{1}{2}}
\]

(2.17)

\[
= \sqrt{2} \left( \frac{\Delta V'}{1 + \frac{dp}{dx}^2} - \frac{1}{2} - \frac{dp}{dx} + \frac{1}{4} \right)^{\frac{1}{2}}
\]

(2.18)

\[
= \sqrt{2} \left( \frac{V'' - \frac{1}{2} - \frac{dp}{dx}}{1 + \frac{dp}{dx}^2} + \frac{1}{4} \right)^{\frac{1}{2}}
\]

(2.19)

\[
\Delta r = r_{n+1} - r_n = \ln(L_{n+1}/dx_0) - \ln(L_n/dx_0)
\]

(2.20)

\[
= \ln(L_{n+1}/L_n)
\]

(2.21)

So, taking the log of both sides, we get

\[
\Delta r = \ln \left( \frac{2 \left( V'' - \frac{1}{2} - \frac{dp}{dx} \right)^2 + \frac{1}{2}}{1 + \frac{dp}{dx}^2} \right)^{\frac{1}{2}}
\]

(2.22)

\[
= \frac{1}{2} \ln \left( \frac{2 \left( V'' - \frac{1}{2} - \frac{dp}{dx} \right)^2 + \frac{1}{2}}{1 + \frac{dp}{dx}^2} \right)
\]

(2.23)
Letting $\frac{dp}{dx} = m$,

$$\Delta r = \frac{1}{2} \ln \left( \frac{2 \left( V'' - \frac{1}{2} - m \right)^2 + \frac{1}{2}}{1 + m^2} \right) \quad (2.24)$$

Because the change in the length is small, the argument of the log is very close to one. In this regime, $\ln(x) \approx x - 1$.

$$\Delta r \approx \frac{1}{2} \left( \frac{2 \left( V'' - \frac{1}{2} - m \right)^2 + \frac{1}{2}}{1 + m^2} - 1 \right)$$

$$\approx \frac{1}{2} \left( \frac{2 \left( V'' - \frac{1}{2} - m \right)^2 + \frac{1}{2} - 1 - m^2}{1 + m^2} \right)$$

$$\approx \frac{1}{2} \left( \frac{2 \left( V'' - \frac{1}{2} V'' - mV'' - \frac{1}{2} V'' + \frac{1}{4} m - mV'' + \frac{1}{2} m + m^2 + \frac{1}{4} - \frac{1}{2} - \frac{1}{2} m^2 \right)}{1 + m^2} \right)$$

$$\approx \left( \frac{V''^2 - V'' + m - 2mV'' + \frac{1}{2} m^2}{1 + m^2} \right) \quad (2.25)$$

the slope $m$ is small so $(1 + m^2)^{-1} \approx 1 - m^2$

$$\Delta r \approx V''^2 - V'' + m - 2mV'' + \frac{1}{2} m^2 \quad (2.26)$$

If $V''$ and $m$ are small,

$$\Delta r \approx m - V'' \quad (2.27)$$
If we ignore the second term for now, as we may, for instance, when $m$ is comparable to or larger than the critical slope, we discover that the rarefaction is simply the integral of the slope with respect to time. Recall that the slope behaves like $m \frac{1}{t - t_c}$ once the critical slope has been exceeded, where $t_c$ is the time at which a caustic is encountered; this implies that the rarefaction should behave like $r \ln(t - t_c)$, which is indeed what we have observed.

Also of note is the fact that equation (2.27) is simply $\Delta r = m + \dot{m}$ for $m << m_{\text{crit}}$.

2.10 Curvature

The density at a point below a caustic will also depend on the curvature of the hairpin in phase space. We begin with three infinitessimally spaced points, labeled as shown in Figure 2.10:

$$\alpha = (x - dx_1, p - dp)$$  \hspace{1cm} (2.28)
$$\beta = (x, p)$$  \hspace{1cm} (2.29)
$$\gamma = ((x + dx_2, p + dp))$$  \hspace{1cm} (2.30)

After a single kick and a single drift, the evolved points are given by

$$\alpha' = (x + p - dx_1 - dp - V'_1, p - dp - V'_1)$$  \hspace{1cm} (2.31)
$$\beta' = (x + p - V', p - V')$$  \hspace{1cm} (2.32)
$$\gamma' = (x + p + dp + dx_2, p + dp - V'_2)$$  \hspace{1cm} (2.33)

as shown in Figure 2.11.
Figure 2.10: Three infinitessimally spaced points.

Figure 2.11: Three infinitessimally spaced points evolved one step.
Let $m_2 = \frac{dp}{dx_2}$, $m = \frac{dp}{dx_1}$. The original curvature is given by

$$c = \frac{\frac{dp}{dx_2} - \frac{dp}{dx_1}}{dx_2} = \frac{m_2 - m}{dx_2}. \quad (2.34)$$

After a single iteration of the map, the curvature is given by

$$c' = \frac{m'_2 - m'}{dx'_2} \quad (2.35)$$

In terms of the new points, this is

$$c' = \frac{\frac{dp - V'_2 + V'}{dp + dx_2 - V'_2 + V'} - \frac{\frac{dp + V'_1 - V'}{dx_1 + dp + V'_1 - V'}}{dp + dx_2 - V'_2 + V'}}{dx'_2} \quad (2.36)$$

$$= \frac{1}{dx_2} \left( \frac{m_2 - V'_2}{m_2 + 1 - V'_2} - \frac{m - V''}{1 + m - V''} \right) \quad (2.37)$$

$$c' - c = \frac{1}{dx_2} \left( \frac{m_2 - m - V''}{m_2 + 1 - V''} - \frac{m - V''}{1 + m - V''} - (m_2 - m) \right) \quad (2.38)$$

$$= \frac{1}{dx_2} \left( \frac{m_2 - m - V'' + V''}{(m_2 + 1 - V'')^2(1 + m - V'')} - m_2 + m \right)$$

If everything is small compared to 1, then this is

$$c' - c \approx \frac{1}{dx_2} \left( (m_2 - m - V'' + V'')(-2m_2 + 1 + 2V'')(1 - m + V'') \right) \quad (2.39)$$

$$-m_2 + m \quad (2.40)$$
Keeping only up to order 2,

\[ dx_2(e' - c) \approx V'' - V''_2 + 4m_2V'' - 2m_2^2 - mV'' + mm_2 \]
\[ -2V''_2^2 + V''_2 - V''m_2 - 2mV'' + m^2 + V''^2 \]

### 2.11 Periodic Branched Flow

One might ask what happens to branches if the random potential is periodic— that is, the potential is random for some interval of time \( \Delta t \) and then repeats the same random sequence. I briefly investigated this, and applied a periodic kick and drift map to both a manifold of classical trajectories and a quantum plane wave. The flow pattern for a manifold of classical trajectories with a repeat length of \( \Delta t = 6 \) steps of the kick and drift map are shown in Figure 2.12.

The flow pattern for a quantum plane wave is shown in Figure 2.13. This was done for a variety of repeat lengths, as the calculation for quantum propagation is much faster than for the classical dynamics.

For short enough periods, the potential acts as a waveguide, but as the repeat length is increased, the flow reverts to the typical behavior of a totally random map. This somewhat surprising result may be worth further exploration.

Another topic worth further consideration is the quantum-classical correspondence for branched flow. Tobias Kramer was the first to notice that as \( \hbar \) is reduced, the quantum mechanical branched flow begins to collapse upon the classical trajectories. Figure 2.14 shows a comparison of a full two-dimensional simulation of classical trajectories with a quantum wavepacket launched in an identical potential. The quan-
Figure 2.12: Periodic branched flow of a manifold of classical trajectories
Figure 2.13: Periodic branched flow of a quantum mechanical plane wave for a variety of repeat lengths.
Figure 2.14: A comparison of the density of classical trajectories (left panel) with a wavepacket launched in the same potential and multiplied by $e^{-iE_0 t/\hbar}$ to get the resulting quantum state with energy $E_0$ (right panel). The yellow arrow indicates a branch evident in the classical density that is absent in the corresponding quantum state. Both panels shown full two-dimensional evolution.
tum state was generated by launching a wavepacket and then multiplying it at each timestep by $e^{-iE_0t/\hbar}$, where $E_0$ is the energy of the eigenstate of interest. This yields a quantum state with energy $E_0$.

One striking feature of the example shown in Figure 2.14 is the branch in the classical simulation, indicated by the yellow arrow in the figure, that is not evident in the quantum results.

More work must be done to understand the convergence as $\hbar$ goes to 0.
Magnetic focusing in graphene

In this chapter we discuss research done via conversations with experimentalists in the Westervelt group, who have imaged magnetic focusing in graphene with a scanning gate microscope. The Westervelt group has used similar techniques to image branched electron flow in a two-dimensional electron gas\textsuperscript{31,33} and to image the magnetic focusing of electrons\textsuperscript{1}, and now they’ve adapted their technique in order to image electron flow in graphene.

Besides being the first experiment of its kind on graphene, it has the potential to be groundbreaking in the realm of transistors. Because graphene is an incredibly fast conductor, if graphene could be used as a transitor it could have the ability to vastly improve current technology. One could imagine using the setup in the experiment
with the tip voltage acting as the “gate” of the transistor, allowing or preventing current from flowing from one lead to another. Using graphene to make an ultrafast device is an attractive idea and is certainly worth exploring.

3.1 The Experiment

The experimental setup is as follows. A Hall bar consisting of a flake of graphene between two layers of 30 nm deep boron nitride is exposed to an external magnetic field. The graphene flake used in the experiment is 4 microns tall by 3 microns wide, and has 6 electrical contacts: one across the top, one across the bottom, and four “legs” with a contact width of 700 nm, as seen in Figure 3.1. These contacts are separated by a center to center distance of 2 microns. The mean free path of the sample is on the order of a few microns. While exposed to the external magnetic field, current is injected into Lead 1 via a current source and the voltage is measured between
Lead 3 and Lead 4 (see Figure 3.1). The experimentalists have found that Lead 4 is essentially at ground voltage. A cooled negatively charged scanning probe microscope tip is kept 20nm above the sample and is then rastered over the flake. The relative change in voltage due to the tip is recorded for each tip location. A voltage difference between Leads 3 and 4 is induced by a current flowing from Lead 1 to the grounded lead. The absolute transresistance is defined to be this measured voltage difference divided by the input current,

$$R_T = \frac{V}{I_{in}}.$$  \hspace{1cm} (3.1)

To isolate the effect of the tip, they subtract the transresistance in the absence of the tip from the absolute measured value. Thus the experiment measures the increase in transmission or decrease in transmission from Lead 1 to Lead 3. The experiment was repeated for a range of magnetic fields and for a range of background carrier densities supplied by a voltage on the backgate. The results of the experiment can be found in the manuscript by the Westervelt group\textsuperscript{5}.

Increasing the background density and increasing the magnetic field have roughly the same effect- hence the diagonal feature in the experimental results.

Let’s first consider what happens in the experiment without the scanning gate microscope tip. When electrons are injected into Lead 1, the applied magnetic field bends the current downward via the Lorentz force. As the magnetic field is increased, the electron’s cyclotron diameter decreases. When the cyclotron diameter for the electrons is equal to the spacing between Leads 3 and 4, a spike in transmission is recorded, as the current is essentially being shot direction into Lead 3 from Lead 1. When the field is reduced such that the cyclotron diameter is about half of the spacing between the leads, another spike, albeit a smaller one, is again recorded. This is
expected assuming that the current is reflected from the edge of the flake between the leads. In fact, theoretically, a spike in transmission should be recorded whenever the spacing between the leads is an integer multiple of the cyclotron diameter.

Measuring the voltage between Leads 3 and 4 as the tip is rastered over the sample leads to a spatial map of the current, although it is not immediately obvious what the correspondence is between the measured transresistance and the value of the current at the present location. For most values of the magnetic field, there are places on the sample where placing the tip dramatically increases the transresistance of the sample and places where it dramatically decreases the transresistance of the sample.

The experimental results, which can be found in the pending publication by the Westervelt group, show a dramatic shift in the spatial pattern of transresistance as the field sweeps through the first focusing field. At lower values of the magnetic field, transresistance is enhanced for tip positions in a curved region outside the cyclotron diameter, and is reduced for tip positions within the cyclotron radius. At higher values of the fields, this behavior is inverted. This makes some intuitive sense, but we can take a closer look at what’s happening by using classical ray tracing.

3.2 Theory

Even in quantum mechanical systems, intuition can be gained by looking at the classical dynamics of individual particles. This is the approach we take here.

In graphene, the dynamical mass of collectively excited electrons has been shown to depend on the carrier density $n$ as $m^* = \hbar \sqrt{\pi n} / v_F$. We argue that this is the dominant effect on the motion of the electrons in the experiment. Since the background carrier electrons can rearrange due to the tip, the electric field from the tip is always perpendicular to the surface of the graphene. Therefore, the electrostatic force
from the tip does not contribute to the force on the electrons. There is also an electric field that arises from the imposed voltage difference between Lead 1 and Lead 2; however, this will be negligible compared to the effect of the applied magnetic field because of the 10 MΩ resistor. The only force the electrons “feel”, therefore, is the force arising from the spatial variation in the carrier density caused by the tip.

There are three contributions to the carrier density in this experiment that we have considered in the theory: the spatially constant background density, $n_0$; the density due to the presence of the tip, $n_{\text{tip}}(r)$; and the variation in density due to the edge effect\(^7\), $n_{\text{edge}}$. This gives an overall carrier density of

$$ n(r) = n_0 + n_{\text{tip}}(r) + n_{\text{edge}}(r). \quad (3.2) $$

Before introducing the magnetic field, we treat the electron as a free particle with a position dependent mass. To find the equations of motion and thus the effective force on the particle, we’ll start with the Lagrangian. Applying the Lagrangian formalism we can determine the force arising from the spatially dependent mass. The Lagrangian for our particle is $\mathcal{L} = \frac{1}{2}m(r)\dot{r}^2$. Applying the Euler-Lagrange equation

$$ \frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} = 0 $$

yields the equation of motion

$$ \frac{1}{2} \nabla m(r)\dot{r}^2 - \left[ \frac{\partial}{\partial t} + \dot{\mathbf{r}} \cdot \nabla \right] (m(r)\dot{r}) = 0 \quad (3.3) $$

$$ \frac{1}{2} \nabla m(r)\dot{r}^2 = m(r)\ddot{r} + \dot{\mathbf{r}} \cdot \nabla m(r) \quad (3.4) $$
where \( m(\mathbf{r}) = \frac{\hbar v_F}{e_F} \sqrt{n(\mathbf{r})} \). Rewriting the equation for clarity gives

\[
\mathbf{\ddot{r}} = \frac{\mathbf{r}^2}{m(\mathbf{r})} \left[ \frac{1}{2} \nabla m(\mathbf{r}) - \left( \mathbf{\dot{r}} \cdot \nabla m(\mathbf{r}) \right) \mathbf{\dot{r}} \right].
\] (3.5)

The first term above represents a force in the direction of the gradient of the mass, while the second term modifies the component of the force in the direction of the velocity. While the first term is intuitive based on the understanding that the tip is repulsive, the second term says that if the particle has a component of its velocity perpendicular to the gradient, the particle will get pulled toward the region of higher density. The effect is that the particle curves toward areas with higher carrier density in the same way that light bends toward regions in a material with higher indices of refraction.

The Lorentz force from the magnetic field simply leads to an additional term, \( \mathbf{\dot{r}}_B = e\mathbf{\dot{r}} B_z/m(\mathbf{r}) \), where the mass again depends on the carrier density. This makes the final equation of motion

\[
\mathbf{\ddot{r}} = \frac{\mathbf{r}^2}{m(\mathbf{r})} \left[ \frac{1}{2} \nabla m(\mathbf{r}) - \left( \mathbf{\dot{r}} \cdot \nabla m(\mathbf{r}) \right) \mathbf{\dot{r}} \right] + e\mathbf{\dot{r}} B_z/m(\mathbf{r}).
\] (3.6)

### 3.2.1 An Equivalent Derivation

In graphene, electrons have been shown to behave like relativistic particles near the Dirac point because of the linear dispersion relation. By treating the flow of electrons as a light wave propagating through a medium with varying index of refraction, we can rederive the same result that we achieved by assuming a spatially dependent mass in the previous section.

To get an equation of motion for ray tracing, we need to find the equation of mo-
tion for the propagation of a single point on the wavefront. We use the Eikonal approximation to get this equation of motion for a particle.

To find the force on the massless particle from the tip, we assume that the electronic density and hence the effective index of refraction changes little over a wavelength. The Helmholtz equation reduces to

\[
\left[ \nabla^2 + \frac{\omega^2}{c^2} n^2(r) \right] \psi = 0. \tag{3.7}
\]

The solutions are locally plane waves, with the form \( \psi = e^{i\omega S(r)/c} \), where \( S(r) \) is the eikonal. Combining these equations and neglecting the higher order term, we have the eikonal approximation,

\[
\nabla S \cdot \nabla S = n^2(r). \tag{3.8}
\]

\[
n(r) \frac{dr}{ds} = \nabla S \tag{3.9}
\]

which leads to a generalization of Snell’s law\(^{15}\),

\[
\frac{d}{ds} \left[ n(r) \frac{dr}{ds} \right] = \nabla n(r). \tag{3.10}
\]

Expanding and using \( d/ds = \hat{k} \cdot \nabla \) and \( dr/ds = \hat{k} \),

\[
\left[ \hat{k} \cdot \nabla n(r) \right] \hat{k} + n(r) \left[ \hat{k} \cdot \nabla \hat{k} \right] = \nabla n(r). \tag{3.11}
\]

Using \( \hat{k} = n(r) \mathbf{v} / c_F \),

\[
2n(r)^2 [\mathbf{v} \cdot \nabla n(r)] \mathbf{v} + n(r) [\mathbf{v} \cdot \nabla \mathbf{v}] = c_F^2 \nabla n(r) \tag{3.12}
\]
Figure 3.2: Trajectories that can get from lead 1 to lead 3 for an ideal point source and drain. There are only two ways from a geometrical perspective: a left adjusted circle (solid lines) or a right adjusted circle (dashed lines) for all radii that are larger than the spacing between the leads. For lower values of the magnetic field, where the cyclotron radius is smaller than the spacing, no trajectories can make it from lead 1 to lead 3.

Now, \( \frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \), but when this acts on \( \mathbf{v} \), which has no explicit time dependence, we get that \( \frac{d\mathbf{v}}{dt} = (\mathbf{v} \cdot \nabla)\mathbf{v} \). Solving for the acceleration, we have finally

\[
\frac{d^2 \mathbf{r}}{dt^2} = c_F^2 \left( \frac{\nabla n(\mathbf{r})}{n(\mathbf{r})^3} \right) - 2 \left( \frac{\mathbf{v} \cdot \nabla n(\mathbf{r})}{n(\mathbf{r})} \right) \mathbf{v}. \tag{3.13}
\]

We note that this is identical to the results from the Lagrangian treatment since \( m(\mathbf{r}) \propto n(\mathbf{r}) \).

3.3 Experimental geometry

In the experiment, the size of the leads is comparable to the spacing between the leads. This has a huge effect on the results. Let’s start by considering a point source and a point drain. In this case, there are exactly two distinct trajectories that can make it from lead 1 to lead three. These correspond to circles whose centers are adjusted to the left and to the right of the wall, so that the circle intersects both contacts. These trajectories are show in Figure 3.2, where the point source is located on the left edge.
at a value of 1 and the point drain is located on the left edge at a value of $-1$.

As the lead is widened and the trajectories get a bit more wiggle room, these two trajectories are “smeared” into many trajectories, but distinct left and right circles as shown in Figure 3.3 remain visible. This figure was made by launching trajectories and integrating their paths via a simple fourth order Runge Kutta method, and then we plot a two-dimensional spatial histogram of only the trajectories that successfully make it to Lead 3 (in other words, we ignored any trajectories that hit a wall).

For leads matched to the experiment, the trajectories launched from the lead are shown in Figure 3.4. If we keep only those trajectories that terminate on Lead 3, the trajectories look much more like a typical cyclotron path, Figure 3.5.

3.4 The Simulation

To understand the effect of the tip in the experiment, we can do some classical trajectory simulations to see what’s really going on. To simulate the experiment, we’ll inject many particles for each tip position, tracing their paths along the way. By raster scanning our “tip” across the sample, we can reconstruct the experiment by keeping track of the particles that successfully travel from Lead 1 to Lead 3.

For each tip position, 10,000 particles with equal energies are injected into the sample from Lead 1. The initial $y$ position of the particles is uniformly distributed over lead 1 and the initial direction of the velocity obeys a cosine distribution around the positive $x$ direction. This equation of motion was integrated numerically using a simple fourth order Runge-Kutta method.

Particles that enter Lead 3 are counted with various weighting, discussed later, and the total is denoted $n_3$. Trajectories that collide with an edge or another lead are terminated. (Extensive simulations were performed with specular and non-specular, or
Figure 3.3: These are two-dimensional spatial histograms only of trajectories that make it from Lead 1 to Lead 3. The contacts here are only 200 nm wide.
Figure 3.4: Showing density of classical trajectories launched as described from lead 1 with no tip present.
Figure 3.5: A plot where we’ve only displayed trajectories that make it from lead 1 to lead 3, without a tip present. As theorists, we get to see what’s actually happening without interrupting the system with a measurement!
random, reflection boundary conditions from the wall. However, the results of those simulation did not bear a particularly strong resemblance to the experimental results, so we choose to terminate at the boundary of the sample.) We also must normalize by the number of particles that would have contributed to $n_3$ without the tip present—let’s denote this $n_0$. The color on the plots is given by

$$\bar{R} = \frac{n_3 - n_0}{N}$$  \hspace{1cm} (3.14)

Where $N$ is the total number of injected particles.

We can simply count the number of trajectories that make it from Lead 1 to Lead 3, or we can weight the particles appropriately. To include the effect of the mean free path, we multiply the contribution from each particle that makes it to lead three by an exponential, so that the total value is given by

$$n_{\text{tot}} = \sum_{i}^{N} e^{-l_i/l_{\text{mfp}}}$$  \hspace{1cm} (3.15)

where the sum is over the trajectories that reach Lead 3, and $l_i$ is the path length of the $i$th trajectory.

The effect of the tip on the carrier density is modeled\textsuperscript{32} as a circularly symmetric lump with the form

$$\sigma(\rho) = \frac{-qa}{2\pi (\rho^2 + a^2)^{3/2}}$$  \hspace{1cm} (3.16)

where $q$ is the charge on the tip, $a$ is the distance from the tip to the surface of graphene, and $\rho$ is the distance to the center of the induced charge distribution. This function has a full width at half maximum of $2\rho_{\text{half max}} = 2a\sqrt{2^{2/3} - 1}$ and the maximum value of the function is $\sigma_{\text{max}} = \frac{-q}{2\pi a^2}$. In the simulation, the tip creates a region of
depletion in the carrier density of about $10^{11}$ cm$^2$.

Simulations were carried out in MATLAB on Harvard University’s Faculty of Arts and Sciences’ supercomputer, the Odyssey Cluster.

3.5 Results

The results of the simulation using both methods of counting trajectories are shown in Figure 3.7 and Figure 3.8, where the images only show the field of view of the experiment. A sample of what this means is shown in Figure 3.6.

Simply counting trajectories reveals a trace of the right adjusted circle, which is not evident in the experiment. Imposing an exponential decay in the weight of each particle due to the mean free path reduced the evidence in the figures of the right-adjusted circles. This makes sense, since particles following those paths would have to travel significantly farther than particles following the left-shifted circles. In the experiment, if the mean free path is short enough, the right adjusted circle would not be able to be seen, as those trajectories are longer and have more of a chance of being kicked off their path.

While the experimental parameters are that the full width half maximum of the carrier density induced by the tip is about 120 nanometers and that there are approximately one hundred electrons on the tip, these parameters produced simulation results with very fine features.

The results of the simulation shown in Figure 3.7 have good qualitative agreement with the experiment; the regions of enhancement of transresistance switch places with the regions of reduction in transresistance around the value of the magnetic field where the cyclotron diameter is equal to the center-to-center spacing between the leads. This makes intuitive sense. A major difference between the experiment and
Figure 3.6: The dynamical mass simulation with $B = 0.12T$, $n = 10^{12}$cm$^{-2}$ with the experimental field of view. The black outline represents the edge of the graphene flake. Areas of the flake that are not scanned by the tip are shown in white. This is an example of the results of the simulation without an imposed mean free path. In other words, all trajectories that reach lead 3 are equally weighted. The crosshairs denote tip locations for the trajectory plots shown elsewhere.
the simulation is that the abruptness with which the regions in the experiment change from increased to decreased transresistance is not reflected in the results of the simulations. The experiment shows high intensity for both regions over a large range of magnetic fields. This also does not seem to be reflected in the simulation results, especially for high magnetic field values. Here, the experiment shows strong regions in which the tip reduces transmission, but the numerical calculations show a weak region with a fairly different shape. One possible explanation is that fluctuations in the background density in the form of “puddles” of electrons or holes dramatically change the trajectories\textsuperscript{22,39}, and we have not taken these into account.

Regardless of the differences, the fact that there is good qualitative agreement is evidence that the phenomenon is mostly classical in nature, and that intuition can be gained for the experiment via a classical mindset.

3.6 Interpreting the Image

If this experiment is to be used for imaging the cyclotron radius, we must understand which part of the image represents the cyclotron orbit. Since the size of the leads is not small in relation to the spacing between the leads, interpreting what represents the actual cyclotron orbit is not as trivial it may at first glance appear.

For a first pass, let’s consider whether the experiment is measuring a picture of the flow. To measure the system, the tip must interact with the sample, and so we shouldn’t expect the conductance to be exactly like the flow without the tip. A simulation showing the flow without the tip is shown in Figure 3.4. No clear cyclotron orbit is present, and the largest density occurs where the manifold of trajectories encounters a caustic. This forms the curved triangular region of higher density in the figure. This is not seen in the experimental results. Now let’s consider the flow of
Figure 3.7: Simulation results for a huge tip on the order of 500nm. The background density is $10^{12} \text{cm}^{-2}$. Transmission was calculated in this case by simply counting the number of particles that made it to lead three. One can see that there is some mark of the larger, right justified cyclotron radius that is not evident in the experiment, ostensibly due to the mean free path of the sample, which is on the order of 2 microns.
Figure 3.8: Same results as Figure 3.7 except that the trajectories are weighted by the distance traveled. One can see that this leaves much less of an imprint of the right justified circle, as those trajectories must travel considerably farther.
Figure 3.9: Showing density of classical trajectories launched as described from lead 1 with the tip at $x = 1\mu m, y = 0$. 
trajectories with the tip present. These are shown in Figure 3.9. Again, no clear cyclotron orbit is present, and there is still a curved triangular region of higher density where the trajectories encounter a caustic. It is possible to see the shadow of the tip in these images.

As these images of the flow do not resemble the experiment, this tells us that the experiment is not reproducing an exact image of the flow, as expected. Let’s consider only the trajectories in these flows that successfully make it from Lead 1 to Lead 3. The trajectory density in this case without the tip is shown in Figure 3.5 and Figure 3.7. Figure 3.5 shows classical trajectories only for those trajectories that end on Lead 3. Other trajectories are not plotted, and there is no tip present anywhere in the system. Compare that to Figure 3.7, which shows the transmission relative to the baseline for each position of the tip. For a magnetic field of 0.13 T, the trajectory plot shows an interior region, absent of any trajectories, with a width of about 0.6 microns. As the magnetic field is reduced, the width of this interior region decreases. This pattern also happens in the interior region of enhanced transresistance in the plot of transmission, shown in Figure 3.7. In fact, this tiny interior region that is absent of trajectories is present over the whole range of the trajectory plots, and it corresponds very well to the ever smaller and smaller interior enhanced region in the transmission plots.

For the larger values of the magnetic field, the reduced region in the transmission plots actually lines up with the outer edge of the trajectories shown in Figure 3.5, and the enhanced region corresponds to the region just outside of the zone of trajectories.

For the value of the magnetic field corresponding to the “first focusing” field, around \( B = 0.10T \), the transmission plot looks qualitatively different than the others in that the region of reduced transresistance is not particularly homogenous in the interior.
Figure 3.10: Spatial histogram of only the trajectories that successfully make it from Lead 1 to Lead 3. The contacts here are only 200 nm wide and the tip is present.
Looking at the trajectory plots, we see that this is where, of course, the two circles we discussed earlier coalesce.

The regions of reduced transresistance in the figure represent areas that would have entered the second lead but were deflected elsewhere by the tip. That is, the reduced regions are trajectories that, under a small perturbation, are knocked out of the lead. These must be the marginal trajectories; those that were just making it into the lead in the absence of the tip.

The enhanced region, on the other hand, represents trajectories that would not have entered Lead 3 without the tip. They are on the other end of the trajectories, the marginal ones that get knocked in with the tip present. By the mean value theorem applied to a continuous manifold of trajectories in phase space, the trajectories between the enhanced and reduced regions must be the ones that are making it squarely with room to spare at Lead 3, so that the modification in their trajectories by the tip just causes the trajectory to enter Lead 3 at another location.

Another explanation could be that in certain areas the tip knocks out just as many particles as it helps funnel into the lead.

We can see by comparing Figure 3.5 with Figure 3.8 that in general, the images are not trivially one-to-one. In particular, if the tip is placed in the center of the electron flow as in Figure 3.10, the particles are deflected, but, because of the geometry and the finite size of the leads, they will still enter the drain! In other words, the tip, with these parameters, anyway, does not directly image the flow of current, but in the limit of point sources and drains, it should.

Another subtlety to keep in mind is the change in the shape of the particle’s orbit due to the increased carrier density along the edge of the sample. Because the density is higher, the orbit will not be perfectly circular, even without the presence of the tip.
In general, it will be shaped more like a horseshoe than a semicircle.

3.7 Discussion

One might ask why the high magnetic field images are so clean and the lower magnetic field ones have so much detail. The answer is that for high values of the magnetic field, where the cyclotron diameter is large enough to make it from one lead to the other for certain intial conditions but not when launched in the positive \(x\) direction from the center of Lead 1, there is essentially only one way for the particle to get from Lead 1 to Lead 3 and all the trajectories between the two extremes also make it from Lead 1 to Lead 3.

For smaller values of the magnetic field, there are other options. Say for example that we inject the particles from a point source and also collect the particles at a point. For a cyclotron diameter greater than the spacing between the source and the drain, there are exactly two initial conditions that will make it from the input to the output, as show in Figure 3.2. As the diameter reduces with increasing field, the two circles converge until we’re left with the circle whose diameter is exactly equal to the spacing between the source and drain.

For perfect point sources and drains, no input particles would make it to the drain for weak tip strengths. However, when we widen the leads we can have diameters that are smaller than the center-to-center spacing yet still can make it from the source to the drain. This case is shown in Figure 3.5 and in Figure 3.8, and we can see that in this case the region of reduced transresistance will have to be simply connected.
3.8 Conclusion

In conclusion we find that care must be taken in interpreting the images formed by measuring the electron flow in this way. It is not always trivial what we’re seeing when we get a high or low reading for the transresistance. In the limit that the lead widths get small compared to the spacing between the leads, the correspondence between the measured transresistance and the electron flow density should get better and better, as the flow is not simply diverted from one part of the lead to another.
Third order thawed gaussian approximation

Semiclassical propagation methods are useful analytic tools and numerical tools. They were important, for example, in proving the existence of scarred eigenfunctions in chaotic systems around classical isolated periodic orbits. In this chapter we will take Heller’s thawed Gaussian approximation\textsuperscript{10} to third order, to better capture the curvature of phase space.

Previous work in semiclassical propagation methods involving Gaussians has relied
on the stability matrix to give instructions to the wavepacket on how to propagate. The stability matrix is a linearization of the phase space dynamics around a point - an expansion of second order. In this approximation, the wavefunction’s center can move and the wavefunction’s width can change, but it will remain Gaussian forever; in the classical phase space, an initially Gaussian distribution can stretch and flatten, but the change in shape is restricted to the linear regime and thus the only shape that can be achieved in phase space for an initially circular distribution is an ellipse.

The real dynamics of a swarm of particles in phase space do not in follow this linear paradigm for most systems. In particular, for chaotic systems a swarm of trajectories can develop curvature very quickly, and there is no way that a linearized Gaussian will maintain good overlap with the true wavefunction.

The beauty of the thawed Gaussian approximation is that an entire wave packet can be propagated by following a single classical trajectory through the system. The thawed Gaussian approximation will, however, fail for highly nonlinear systems or for very long times of propagation, for exactly the reason described above- the Gaussian cannot capture curvature in phase space.

It is logical that expanding the thawed Gaussian approximation to third order would yield a better result. In particular this approach will allow our evolving wave packet to develop asymmetry in both space and momentum, whereas in the original second order thawed gaussian approximation the initial Gaussian wavepacket is always propagating in a harmonic potential and will therefore remain symmetric for all time. The tradeoff of this approach is that we will have to do a bit more work but will still only have to run a single trajectory.

Like the thawed Gaussian approximation, where an initial Gaussian wave function is propagated essentially under a harmonic potential with a time dependent width,
here we are propagating our function under a time dependent cubic potential that approximates the real potential near the central guiding trajectory. This should capture some of the curvature of phase space.

This chapter details the steps needed to derive the third order thawed Gaussian approximation. Work must still be done to implement it numerically in an efficient manner, as the closed form solutions are currently intractable.

4.1 THAWED GAUSSIAN APPROXIMATION

Let’s begin with a discussion of the original work on thawed Gaussians by Heller.

\[
\Psi_{\beta}^{\text{lsc}}(q, t) = \int dq' G^{\text{lsc}}(q, q', t) \Psi_{\beta}(q', 0),
\]

(4.1)

where

\[
G^{\text{lsc}}(q, q', t) = \frac{1}{\sqrt{2\pi i \hbar}} \sum_{\text{paths}} \left| \frac{\partial^2 S(q, q')}{\partial q \partial q'} \right|^{1/2} \exp \left[ i S^{\text{lin}}(q, q', t) \right].
\]

(4.2)

4.2 THE THIRD ORDER EXPANSION

We start by expanding the action \( S(q, q') \) to third order around the endpoints in position space, \( q_0 \) and \( q_t \). This gives
\[ S^{\text{cube}}(q, q') = S(q_t, q_0) + \left( \frac{\partial S}{\partial q_t} \right)_{q_0} (q - q_t) + \left( \frac{\partial S}{\partial q_0} \right)_{q_t} (q' - q_0) \]

\[ + \frac{1}{2} \left( \frac{\partial^2 S}{\partial q_t^2} \right)_{q_0} (q - q_t)^2 + \frac{1}{2} \left( \frac{\partial^2 S}{\partial q_0^2} \right)_{q_t} (q' - q_0)^2 \]

\[ + \frac{1}{6} \left( \frac{\partial^3 S}{\partial q_0^3} \right)_{q_t} (q' - q_0)^3 + \frac{1}{2} \left( \frac{\partial^3 S}{\partial q_0^2 \partial q_t} \right)_{q_0} (q - q_t)^3 \]

\[ + \frac{1}{2} \left( \frac{\partial^3 S}{\partial q_0^2 \partial q_t} \right)_{q_0} (q - q_t)(q' - q_0)^2 + \frac{1}{2} \left( \frac{\partial^3 S}{\partial q_0 \partial q_t^2} \right)_{q_t} (q - q_t)^2(q' - q_0). \]

Applying Equation 4.4 to the propagator we get

\[ \Psi^{\text{sc}}_{\beta}(q, t) = N \frac{1}{\sqrt{2\pi i\hbar}} \sum_{\text{paths}} \int dq' \left| \frac{\partial^2 S}{\partial q_0 \partial q_t} + \left( \frac{\partial^3 S}{\partial q_0^2 \partial q_t} \right) (q' - q_0) \right. \]

\[ + \frac{1}{2} \left( \frac{\partial^3 S}{\partial q_0 \partial q_t^2} \right) (q - q_t) \left|^{1/2} \right. \]

\[ \times \exp \left\{ i \left[ \Xi q' + \Upsilon q'^2 + \Omega q' + \Lambda \right] \right\} \]

where
\[
\Xi = \frac{1}{6} \left( \frac{\partial^3 S}{\partial q_t^2} \right)_{q_t}, \quad (4.5)
\]

\[
\Upsilon = \frac{1}{2} \left[ \left( \frac{\partial^2 S}{\partial q_0^2} \right)_{q_t} + \left( \frac{\partial^3 S}{\partial q_0^2 \partial q_t} \right) q - \left( \frac{\partial^3 S}{\partial q_t^2} \right) q_t - \left( \frac{\partial^3 S}{\partial q_0^2 \partial q_t} \right) q_0 \right] + A, \quad (4.6)
\]

\[
\Omega = \left( \frac{\partial S}{\partial q_0} \right)_{q_t} + \left( \frac{\partial^2 S}{\partial q_0 \partial q_t} \right) (q - q_t) - \left( \frac{\partial^2 S}{\partial q_t} \right) q_0 + \left( \frac{\partial^3 S}{\partial q_0^2 \partial q_t} \right) (q_0 q_t - q q_0)
\]

\[
+ \frac{1}{2} \left( \frac{\partial^3 S}{\partial q_0^2} \right) q_0^2 + \left( \frac{\partial^3 S}{\partial q_0 \partial q_t^2} \right) \left( \frac{1}{2} q_t^2 + \frac{1}{2} q^2 - q q_t \right) - 2Aq_3 + \xi, \quad (4.7)
\]

\[
\Lambda = \left( \frac{\partial S}{\partial q_t} \right) q + \frac{1}{2} \left( \frac{\partial^2 S}{\partial q_t^2} \right) q^2 + \frac{1}{6} \left( \frac{\partial^3 S}{\partial q_t^3} \right) q^3 - \left( \frac{\partial S}{\partial q_0} \right) q_0
\]

\[
- \left( \frac{\partial^2 S}{\partial q_0 \partial q_t} \right) q_0 q_t - \frac{1}{2} \left( \frac{\partial^3 S}{\partial q_0 \partial q_t^2} \right) q^2 q_0 + \frac{1}{2} \left( \frac{\partial^2 S}{\partial q_0} \right) q_0^2
\]

\[
+ \frac{1}{2} \left( \frac{\partial^3 S}{\partial q_0^2} \right) q_0 q_t
\]

\[
- \frac{1}{6} \left( \frac{\partial^3 S}{\partial q_0^2} \right) q_0^3 - \left( \frac{\partial S}{\partial q_t} \right) q_t - \left( \frac{\partial^2 S}{\partial q_t^2} \right) q_0 q_t - \frac{1}{2} \left( \frac{\partial^3 S}{\partial q_t^3} \right) q_0^2 q_t
\]

\[
+ \left( \frac{\partial^3 S}{\partial q_0 \partial q_t} \right) q_0 q_t + \left( \frac{\partial^3 S}{\partial q_0 \partial q_t^2} \right) q_0 q_t - \frac{1}{2} \left( \frac{\partial^3 S}{\partial q_0} \right) q_0^2 q_t
\]

\[
+ \frac{1}{2} \left( \frac{\partial^3 S}{\partial q_t} \right) q_0^2
\]

\[
+ \frac{1}{2} \left( \frac{\partial^3 S}{\partial q_t^2} \right) q_0^2 - \frac{1}{2} \left( \frac{\partial^3 S}{\partial q_0 \partial q_t^2} \right) q_0 q_t - \frac{1}{6} \left( \frac{\partial^3 S}{\partial q_t^3} \right) q_0 q_t^2
\]

\[
+ Aq_3^2 + S + \gamma - \xi q_3. \quad (4.8)
\]

### 4.3 Closed-Form Solution

For the purposes of efficient numerical implementation, it is important that we find a tractable closed-form solution to the integral in Equation 4.5. We will begin by focus-
ing on the phase $\phi$ in the exponential in Equation 4.5 where

$$\Psi_{\beta}^{bc}(q, t) = N \frac{1}{\sqrt{2\pi i\hbar}} \sum_i \int dq' A(q, t) \exp \{i\phi\} ; \quad (4.9)$$

$$\phi = \Xi q'^3 + \Upsilon q'^2 + \Omega q' + \Lambda$$
$$= \Xi \left( q'^3 + \frac{1}{3} \Upsilon q'^2 + \frac{1}{3} \Omega q' + \frac{1}{3} \Lambda \right)$$
$$= \Xi \left[ (q' + \frac{1}{3} \Upsilon) \left( \frac{1}{3} \Upsilon \right)^2 + \frac{1}{27} \left( \frac{1}{3} \Omega \right)^3 + \frac{1}{27} \Upsilon q' + \frac{1}{27} \Lambda \right]$$

$$Let \ t = (q' + \frac{1}{3} \Upsilon).$$

$$\implies \phi = \Xi t^3 + \Xi \left( \frac{1}{3} \Omega - \frac{1}{3} \left( \frac{1}{3} \Upsilon \right)^2 \right) t - \frac{1}{3} \Xi \left( \frac{1}{3} \Omega - \frac{1}{3} \left( \frac{1}{3} \Upsilon \right)^2 \right) - \frac{1}{27} \frac{1}{3} \Upsilon^3 + \Lambda \quad (4.10)$$

Hence,

$$\Psi_{\beta}^{bc}(q, t)$$
$$= N \frac{1}{\sqrt{2\pi i\hbar}} \sum_i \int_{-\infty}^{\infty} dq' \left[ \frac{\partial^2 S}{\partial q_0 \partial q_i} + \left( \frac{\partial^3 S}{\partial q_0^2 \partial q_i} \right) (q' - q_0) \right] \left[ \frac{\partial^3 S}{\partial q_0 \partial q_i} \right] (q - q_i)^{1/2}$$
$$\times \exp \left\{ i \left[ \Xi q'^3 + \Upsilon q'^2 + \Omega q' + \Lambda \right] \right\}$$
$$= N \frac{1}{\sqrt{2\pi i\hbar}} \sum_i \int_{-\infty}^{\infty} dt \left[ \frac{\partial^2 S}{\partial q_0 \partial q_i} \right] \left[ \frac{\partial^3 S}{\partial q_0 \partial q_i} \right] (q' - q_0) \left[ \frac{\partial^3 S}{\partial q_0 \partial q_i} \right] (q - q_i)^{1/2}$$
$$\times \exp \left\{ i \left[ \Xi t^3 + \Xi \left( \frac{1}{3} \Omega - \frac{1}{3} \left( \frac{1}{3} \Upsilon \right)^2 \right) t - \frac{1}{3} \Xi \left( \frac{1}{3} \Omega - \frac{1}{3} \left( \frac{1}{3} \Upsilon \right)^2 \right) - \frac{1}{27} \frac{1}{3} \Upsilon^3 + \Lambda \right] \right\}.$$
We expand the prefactor out with respect to $q'$ using a Taylor Series centred on $q_0$:

$$
\Psi_{\beta}(q,t) = N \frac{1}{\sqrt{2\pi i}} \int_{-\infty + \frac{i}{3}}^{\infty + \frac{i}{3}} dt \sum_{n=0}^{\infty} \frac{(-1)^n (2n)!}{(1-2n)(n!)^2 (4^n)} \left[ \frac{\partial^2 S}{\partial q_0 \partial q_t} + \left( \frac{\partial^3 S}{\partial q_0 \partial q_t^2} \right) (q-q_t) \right]^{\frac{1}{2}-n} \left( \frac{\partial^3 S}{\partial q_0^2 \partial q_t} \right)^n (q' - q_0)^n 
\times \exp \left\{ i \left[ \Xi t^3 + \Xi \left( \frac{\Omega}{\Xi} - \frac{1}{3} \left( \frac{\Upsilon}{\Xi} \right)^2 \right) t - \frac{1}{3} \Xi \left( \frac{\Omega}{\Xi} - \frac{1}{3} \left( \frac{\Upsilon}{\Xi} \right)^2 \right) - \frac{1}{27 \Xi^2} + \Lambda \right] \right\} 
\times \sum_{m=0}^{n} \left( \frac{n}{m} \right) \left( -\frac{1}{3} \frac{\Xi}{\Xi} - q_0 \right)^{n-m} t^m 
\times \exp \left\{ i \left[ \Xi t^3 + \Xi \left( \frac{\Omega}{\Xi} - \frac{1}{3} \left( \frac{\Upsilon}{\Xi} \right)^2 \right) t - \frac{1}{3} \Xi \left( \frac{\Omega}{\Xi} - \frac{1}{3} \left( \frac{\Upsilon}{\Xi} \right)^2 \right) - \frac{1}{27 \Xi^2} + \Lambda \right] \right\}
$$
\[
\begin{align*}
&= N \frac{1}{\sqrt{2\pi i\hbar}} \exp \left\{ -i \left[ \frac{1}{3} \Upsilon \left( \frac{\Omega}{\Xi} - \frac{1}{3} \left( \frac{\Upsilon}{\Xi} \right)^2 \right) + \frac{1}{27} \frac{\Upsilon^3}{\Xi^2} - \Lambda \right] \right\} \\
&\times \sum_{n=0}^{\infty} \frac{(-1)^n(2n)!}{(1-2n)(n!)^2} \left[ \frac{\partial^2 S}{\partial q_0 \partial q_t} + \left( \frac{\partial^3 S}{\partial q_0 \partial q_t^2} \right)(q - q_t) \right]^{\frac{1}{2} - n} \left( \frac{\partial^3 S}{\partial q_0^2 \partial q_t} \right)^n \\
&\times \sum_{m=0}^{n} \binom{n}{m} \left( -\frac{1}{3} \Xi - q_0 \right)^{n-m} \\
&\times \left\{ \frac{1}{6} (-1)^m (i\Xi)^{-\frac{m}{3}} \left[ 2(i\Xi)^{2/3} \Gamma \left( \frac{m+1}{3} \right) {}_1F_2 \left( \frac{m}{3} + \frac{1}{3} ; \frac{1}{3} ; \frac{2}{3} ; \frac{Z^3}{27(i\Xi)} \right) \\
+ Z \left( 2\sqrt{(i\Xi)} \Gamma \left( \frac{m+2}{3} \right) {}_1F_2 \left( \frac{m}{3} + \frac{2}{3} ; \frac{4}{3} ; \frac{Z^3}{27(i\Xi)} \right) \\
+ Z \Gamma \left( \frac{m}{3} + 1 \right) {}_1F_2 \left( \frac{m}{3} + 1 ; \frac{4}{3} ; \frac{5}{3} ; \frac{Z^3}{27(i\Xi)} \right) \right) \right] \\
+ \frac{1}{6} (-i\Xi)^{-\frac{m}{3}} \left[ 2(-i\Xi)^{2/3} \Gamma \left( \frac{m+1}{3} \right) {}_1F_2 \left( \frac{m}{3} + \frac{1}{3} ; \frac{1}{3} ; \frac{2}{3} ; \frac{Z^3}{27(i\Xi)} \right) \\
+ Z \left( Z \Gamma \left( \frac{m}{3} + 1 \right) {}_1F_2 \left( \frac{m}{3} + 1 ; \frac{4}{3} ; \frac{5}{3} ; \frac{Z^3}{27(i\Xi)} \right) \\
- 2\sqrt{-i\Xi} \Gamma \left( \frac{m+2}{3} \right) {}_1F_2 \left( \frac{m}{3} + \frac{2}{3} ; \frac{2}{3} ; \frac{4}{3} ; \frac{Z^3}{27(i\Xi)} \right) \right) \right] \right\}. 
\end{align*}
\]

where
\[
Z = -\Xi \left( \frac{\Omega}{\Xi} - \frac{1}{3} \left( \frac{\Upsilon}{\Xi} \right)^2 \right),
\]

and we used the following identity, based on the Laplace transform, to perform the integral:
\[
\int_{-\infty}^{\infty} x^n e^{\alpha x^3} e^{-px} dx = \int_{0}^{\infty} x^n e^{\alpha x^3} e^{-px} dx + \int_{0}^{\infty} (-x)^n e^{\alpha(-x)^3} e^{-p(-x)} dx \quad (4.12)
\]

\[
= \mathcal{L}_x \left[ x^n e^{\alpha x^3} \right] (p) + \mathcal{L}_x \left[ (-x)^n e^{\alpha(-x)^3} \right] (-p)
\]

\[
= \frac{1}{6} (-1)^n \alpha^{-\frac{n}{3} - 1} \left\{ 2 \alpha^{2/3} \Gamma \left( \frac{n+1}{3} \right) \ _2F_1 \left( \frac{n}{3} + \frac{1}{3}; \frac{2}{3}; \frac{4}{3}; \frac{p^3}{27\alpha} \right) + p \left[ 2 \sqrt{\frac{\alpha}{\Gamma}} \left( \frac{n+2}{3} \right) \ _2F_1 \left( \frac{n}{3} + \frac{2}{3}; \frac{2}{3}; \frac{4}{3}; \frac{p^3}{27\alpha} \right) \right. \right.

\left. + p \Gamma \left( \frac{n}{3} + 1 \right) \ _2F_1 \left( \frac{n}{3} + 1; \frac{4}{3}; \frac{5}{3}; \frac{p^3}{27\alpha} \right) \right\}
\]

\[
+ \frac{1}{6} (-\alpha)^{-\frac{n}{3} - 1} \left\{ 2 (-\alpha)^{2/3} \Gamma \left( \frac{n+1}{3} \right) \ _2F_1 \left( \frac{n}{3} + \frac{1}{3}; \frac{2}{3}; \frac{4}{3}; \frac{p^3}{27\alpha} \right) + p \left[ p \Gamma \left( \frac{n}{3} + 1 \right) \ _2F_1 \left( \frac{n}{3} + 1; \frac{4}{3}; \frac{5}{3}; \frac{p^3}{27\alpha} \right) \right. \right.

\left. - 2 \sqrt{-\alpha} \Gamma \left( \frac{n+2}{3} \right) \ _2F_1 \left( \frac{n}{3} + \frac{2}{3}; \frac{2}{3}; \frac{4}{3}; \frac{p^3}{27\alpha} \right) \right\}.
\]

**4.4 Computation**

We define our stability matrix as

\[
M(t) = \begin{pmatrix}
\frac{\partial p_t}{\partial p_0} \bigg|_{q_1} & \frac{\partial q_t}{\partial q_0} \bigg|_{p_0} \\
\frac{\partial p_t}{\partial q_0} & \frac{\partial q_t}{\partial q_0} \bigg|_{p_0}
\end{pmatrix}.
\]
The generating equation for second order derivatives is

\[ \dot{M}(t) = K(t) \cdot M(t) \]  

where

\[ K(t) = \begin{pmatrix} \frac{\partial^2 H}{\partial q \partial p} & -\frac{\partial^2 H}{\partial q^2} \\ \frac{\partial^2 H}{\partial p \partial q} & \frac{\partial^2 H}{\partial p^2} \end{pmatrix}. \]  

(4.15)

For a general Hamiltonian \( H = \frac{p^2}{2m} + V(q) \),

\[ K(t) = \begin{pmatrix} 0 & -\frac{\partial^2 V(q)}{\partial q^2} \\ \frac{1}{m} & 0 \end{pmatrix}. \]  

(4.16)

The second order derivative are:

\[ \frac{\partial^2 S}{\partial q_0 \partial q_l} = -\frac{1}{M_{21}}, \]  

(4.17)

\[ \frac{\partial^2 S}{\partial q_0 \partial q_0} = \frac{M_{22}}{M_{21}}, \]  

(4.18)

\[ \frac{\partial^2 S}{\partial q_i \partial q_l} = \frac{M_{11}}{M_{21}}, \]  

(4.19)

and \( M(0) = I_{2 \times 2} \).

Similarly, the generating equation for third order derivatives (using Einstein notation) is:

\[ \dot{\Gamma}(t) = \frac{\partial K(t)}{\partial (p, q)_{ij}} M(t)_{kl} M(t)_{jm} + K(t)_{ij} \Gamma(t)_{jm}, \]  

(4.21)
where $\Gamma(t)$ is a $2N \times 2N \times 2N$ tensor that is defined to be $\frac{\partial M}{\partial (p_0, q_0)}$ and

\[
\frac{\partial K(t)}{\partial p} = \begin{pmatrix}
  -\frac{\partial^3 H}{\partial q \partial p^2} & -\frac{\partial^3 H}{\partial q^2 \partial p} \\
  \frac{\partial^3 H}{\partial p^2 \partial q} & \frac{\partial^3 H}{\partial q^2 \partial p}
\end{pmatrix},
\]  \tag{4.22}

\[
\frac{\partial K(t)}{\partial q} = \begin{pmatrix}
  -\frac{\partial^3 H}{\partial q^2 \partial p} & -\frac{\partial^3 H}{\partial q^4} \\
  \frac{\partial^3 H}{\partial p^2 \partial q} & \frac{\partial^3 H}{\partial q^4}
\end{pmatrix}.
\]  \tag{4.23}

For a general Hamiltonian $H = \frac{p^2}{2m} + V(q)$,

\[
\frac{\partial K(t)}{\partial p} = 0 \times I_{2 \times 2},
\]  \tag{4.24}

and

\[
\frac{\partial K(t)}{\partial q} = \begin{pmatrix}
  0 & -\frac{\partial^3 V(q)}{\partial q^3} \\
  0 & 0
\end{pmatrix}.
\]  \tag{4.25}

The third order derivatives are:

\[
\frac{\partial^3 S}{\partial q_0^7} = \frac{1}{M_{21}} \left( \Gamma_{222} - \frac{M_{22}}{M_{21}} \Gamma_{221} \right) - \frac{M_{22}}{(M_{21})^2} \left( \Gamma_{212} - \frac{M_{22}}{M_{21}} \Gamma_{211} \right),
\]  \tag{4.26}

\[
\frac{\partial^3 S}{\partial q_0^7 \partial q_t} = \frac{1}{(M_{21})^2} \left( \Gamma_{212} - \frac{M_{22}}{M_{21}} \Gamma_{211} \right),
\]  \tag{4.27}

\[
\frac{\partial^3 S}{\partial q_0 \partial q_t^2} = \frac{1}{M_{21}} \left( \Gamma_{112} - \frac{M_{22}}{M_{21}} \Gamma_{111} \right) - \frac{M_{11}}{(M_{21})^2} \left( \Gamma_{212} - \frac{M_{22}}{M_{21}} \Gamma_{211} \right),
\]  \tag{4.28}

\[
= \frac{\Gamma_{211}}{(M_{21})^3},
\]  \tag{4.29}

\[
\frac{\partial^3 S}{\partial q_t \partial q_t \partial q_t} = \frac{1}{M_{21}^2} \left( \Gamma_{111} - \frac{M_{11}}{M_{21}} \Gamma_{211} \right).
\]  \tag{4.30}

and $\Gamma(0) = 0 \times I_{2 \times 2 \times 2}$. 

94
4.5 Classical behavior

Like the thawed Gaussian approximation, where an initial Gaussian wave function is propagated essentially under a harmonic potential with a time dependent width, here we are propagating our function under a time dependent cubic potential that approximates the real potential near the central guiding trajectory. This should capture some of the curvature of phase space. An example of the classical results for propagation under the various methods are shown in Figure 4.1.

![Figure 4.1](image.png)

**Figure 4.1:** Contours of a classical distribution of trajectories launched in the quartic potential. The initial Gaussian distributions first confidence interval contour is shown in green, and overlaps with the various methods are shown overlapping the initial state at the first recurrence.

We can see that the contour for the initially Gaussian distribution has remained elliptical under the thawed Gaussian approximation, as it should. The classical distribution evolved under TOTGA has developed a curvature in phase space and closely
matches the true distribution close to the guiding trajectory. Away from the guiding trajectory the distributions are radically different, which is to be expected.

That the classical distribution in phase space is a closer match near the guiding trajectory is promising for implementing the semiclassical propagation.
References


