Semiclassical Scattering for Two and Three Body Systems

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Abstract

Semiclassical scattering theory can be summarized as the study of connections between classical mechanics and quantum mechanics in the limit $\hbar \to 0$ over the infinite time domain $-\infty < t < \infty$. After a brief discussion of Semiclassical Analysis and Scattering Theory we provide a rigorous result concerning the time propagation of a semiclassical wave-packet over the time domain $-\infty < t < \infty$. This result has long been known for dimension $n \geq 3$, and we extend it to one and two space dimensions. Next, we present a brief mathematical discussion of the three body problem, first in classical mechanics and then in quantum mechanics. Finally using an approach similar to the semiclassical wave-packet construction we form a semiclassical approximation to the solution of the Schrödinger equation for the three-body problem over the time domain $-\infty < t < \infty$. This technique accounts for clustering at infinite times and should be applicable for researchers studying simple recombination problems from quantum chemistry.

Contents

Chapter 1

Introduction

Semiclassical mechanics is the study of quantum mechanics in the limit $\hbar \to 0$. Scattering theory is the study of dynamics over infinite time intervals. A basic question of scattering theory is: Given the state of a system at $t = -\infty$, under what conditions can we obtain information about the system at $t = \infty$? In this report we study the semiclassical limit of scattering processes for certain two and three body systems. Much of the material presented here is background material. The bulk of the original material appears in chapters four and six.

Our approach to semiclassical mechanics involves the use of an indexed set of parameterized semiclassical wave-packets $\phi_k(A(t), B(t), \hbar, a(t), \eta(t), x)$ that form an orthonormal basis for $L^2(\mathbb{R}^n)$. We can use these wave-packets to give approximate solutions to the time dependent Schrödinger equation

$$i\hbar \frac{d}{dt}\psi(x, t, \hbar) = -\frac{\hbar^2}{2}\triangle_x \psi(x, t, \hbar) + V(x)\psi(x, t, \hbar). \tag{1.1}$$

Let $a(t), \eta(t)$ be the classical position and momentum for the conservative system with potential $V(x)$. Let $W_{a(t)}(x)$ be the second order Taylor expansion of $V(x)$ about the classical position $a(t)$. The wave-packets give exact solutions to the Schrödinger equation

$$\begin{aligned} & i\hbar \frac{d}{dt}\left\{e^{iS(t)/\hbar}\phi_k(A(t), B(t), \hbar, a(t), \eta(t), x)\right\} \qquad (1.2)\\ = & \left\{-\frac{\hbar^2}{2}\triangle_x + W_{a(t)}(x)\right\}\left\{e^{iS(t)/\hbar}\phi_k(A(t), B(t), \hbar, a(t), \eta(t), x)\right\}. \end{aligned}$$

The parameters $A(t), B(t)$ are variables characterizing the spreading of position and momentum. $S(t)$ is the classical action. We denote the propagator for (1.1) to be $U(t)$ and the propagator for (1.2) to be $U_1(t, 0)$. Our study of semiclassical analysis involves showing that under appropriate conditions

$$\lim_{\hbar \to 0} \|\{U(t) - U_1(t, 0)\}\phi_k(A(0), B(0), \hbar, a(0), \eta(0), x)\|_2 = 0.$$

In general, the above limit is valid for any finite time t. When discussing scattering processes we show that this limit can be taken uniformly in time. In chapter four of this report we show that for the index $k = 0$ this limit is uniform in time if the potential $V(x)$ exhibits sufficient decay. Thus the quantum scattering map can be approximated in the semiclassical limit if the classical scattering map is known.

For two body scattering problems the dynamics is asymptotic to the dynamics of a free system for large times. The three body problem is more complicated since the dynamics for large times might approach a system that is not free. It is well known in both quantum and classical mechanics that under appropriate conditions on the system, the dynamics of a three body system may be asymptotic to states where two of the particles are bound and the third particle is free. In chapter 6 we provide a modification to the semiclassical scheme to account for this situation and show how the classical mechanics of a three body system can be used to provide an approximate solution to the Schrödinger equation. We believe the technique developed in chapter 6 will be useful to researchers studying collinear three body recombination problems. The motivation for the material in chapter 6 is the study of a simple collinear chemical reaction

$$(AB) + C \rightarrow \begin{cases} (AB) + C & \text{No molecular reaction occurs,} \\ A + (BC) & \text{molecular reaction occurs.} \end{cases}$$

The semiclassical approach is appropriate for chemical reactions since the molecular masses are relatively large.

This report is organized as follows: In this chapter we give a brief introduction to classical mechanics and quantum mechanics. In chapter two we describe some classic results from semiclassical analysis and the construction of the semiclassical wave-packets. In chapter three we discuss scattering theory of two body problems. In chapter four we present a result about the scattering of wave-packets in low dimensions. In chapter five we discuss scattering theory for the three body problem. In chapter six we present a semiclassical approximation for the collinear three body problem. In chapter seven we conclude by discussing possible directions that one can take in this line of research.

Throughout we assume that the reader is familiar with standard Hilbert Space Theory and the use of multi-index notation. The inner products that we use are linear in the second argument and conjugate linear in the first argument.

1.1 A brief introduction to Classical Mechanics

Here we provide a very brief introduction to classical mechanics. Suppose that a particle of mass m is governed by a potential $V(x)$, the movement in $\mathbb{R}^n$ is ruled by Hamilton's laws

$$\dot{q}(t) = p(t)/m \tag{1.3}$$

$$\dot{p}(t) = -\nabla V(q(t)). \tag{1.4}$$

In the above $q(t)$ and $p(t)$ are vectors in $\mathbb{R}^n$. The total energy of the system is defined to be

$$E = \frac{p^2(t)}{2m} + V(q(t)). \tag{1.5}$$

It is well known that energy is a conserved quantity for this type of system. Moreover, any observable quantity can be expressed as a function of position and momentum. Suppose $V(x)$ has a global minimum at $x = x_0$ and $\underline{\lim}_{|x|\to\infty} V(x) > V(x_0)$, then $V(x_0)$ is known as the ground state energy. It is a quick matter to see that $E \geq V(x_0)$.

1.2 A brief introduction to Quantum Mechanics

We present next a quick introduction to Quantum Mechanics. A formal discussion of the postulates of Quantum Mechanics is given in [27], the basis of our discussion follows that reference. We warn the reader that we make no pretension that we can provide a complete discussion on the foundations or postulates of quantum mechanics. We overlook many subtleties of the theory in favor of a quick introduction.

The postulates of Quantum Mechanics:

1) The dynamical states $\psi(x,t)$ in Quantum Mechanics are represented by normalized elements of a Hilbert space $\mathcal{H}$, usually $L^2(\mathbb{R}^n)$, where $x \in \mathbb{R}^n$ and t is treated as a parameter.

2) Position and momentum are represented by the self adjoint operators $Q = x$, and $P = -i\hbar\frac{d}{dx}$ respectively. Any observable quantity $\omega(q,p)$ of classical mechanics is represented by the self-adjoint operator $\Omega(q \to Q, p \to P)$. The involved process of representing a classical observable by a quantum observable is known as **quantization**. A common obstacle with quantization is that while the classical variables q and p commute, the observables Q and P don't. To take care of this one can often make the transformation $qp = \frac{1}{2}(QP + PQ)$. The study of quantization is a rich research subject in its own right and so we avoid a more in depth discussion here.

3) If a particle is in a state $\psi(x,t)$, measurement of an observable Ω will generate a real number a in the spectrum of Ω, with corresponding "normalized" generalized eigenvector $\lambda_a(x)$. The value of the observed quantity will be a with probability

$$P_{\Omega_\psi}[a] = |\langle \lambda_a(x), \psi(x,t)\rangle|^2,$$

here $\langle , \rangle$ is the standard inner product on $\mathcal{H}$. Furthermore the expectation value μ_{Ω_ψ} of Ω measured against $\psi(x,t)$ is given by

$$\mu_{\Omega_\psi} = \langle \psi(x,t), \Omega\psi(x,t)\rangle.$$

In the case that $a \in \sigma_{pp}(\Omega)$ then the condition that $\lambda_a(x)$ is normalized is expressed as $\|\lambda_a(x)\|_2 = 1$. If $a \in \sigma_{ess}(\Omega)$ then the normalization condition is expressed formally as $\int_{\mathbb{R}} \lambda_{a'}(x)\lambda_a^*(x)dx = \delta(a' - a)$.

4) The state vector's time evolution is governed by the Schrödinger equation

$$i\hbar \frac{d}{dt}\psi(x,t) = H\psi(x,t).$$

Here H is the self-adjoint operator representing the energy of the system.

At this point we find it convenient to define the **variance** of the measurement Ω by

$$\sigma_{\Omega_\psi}^2 = \langle \psi(x,t), (\Omega - \mu_{\Omega_\psi})^2 \psi(x,t) \rangle.$$

We warn the reader that some authors define the variance to be σ rather than σ^2 as we have.

Chapter 2

Semiclassical analysis

2.1 Introduction to Semiclassical Analysis

Semiclassical analysis is the study of what is known to physicists as the Bohr correspondence principle: In the limit $\hbar \to 0$ quantum mechanics yields classical mechanics. We begin this chapter by stating rigorous results for various folk theorems of quantum mechanics, in particular those regarding eigenvector approximation and exponential decay of eigenfunctions. Next we introduce the semiclassical wave-packets which we use to prove results of semiclassical analysis. Afterwards we state a result about the quasiclassical quantization of bound states.

2.2 Semiclassical Analysis of Bound States

The oldest and most widely known semiclassical approximation is the WKB approximation, sometimes called the JWKB approximation. This semiclassical approximation gives the small $\hbar$ approximation for the bound states of the Schrödinger operator

$$H = -\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + V(x)$$

in one dimension. We present a rigorous result concerning the WKB approximation for the classically acceptable region. Our discussion is based on the one found in [28]. A formal discussion of the WKB approximation can be found in most introductory texts on Quantum Mechanics. We first consider solutions to the time independent Schrödinger equation

$$H\lambda(\hbar; x) - E\lambda(\hbar; x) = 0. \tag{2.1}$$

Lemma 2.2. *Let $E \in \mathbb{R}, V(x) \in C^2[a, b]$ be chosen such that $V(x) < E$ for all $x \in [a, b]$ and suppose there exists a solution to (2.1) in L^2. Then for all $x \in [a, b]$ the solution of (2.1) is* *given by*

$$\lambda(\hbar;x) = C_1(E-V(x))^{-1/4}\exp\left\{i\frac{\sqrt{2M}}{\hbar}\int_{x_0}^{x}\sqrt{E-V(y)}dy\right\}\{1+O(\hbar)\} \quad (2.3)$$
$$+C_2(E-V(x))^{-1/4}\exp\left\{-i\frac{\sqrt{2M}}{\hbar}\int_{x_0}^{x}\sqrt{E-V(y)}dy\right\}\{1+O(\hbar)\}.$$

Proof. Letting $Q(x,E) = E - V(x) > 0$ The Schrödinger equation now becomes

$$\lambda''(\hbar;x) + \rho^2 Q(x,E)\lambda(\hbar,x) = 0 \quad (2.4)$$

with $\rho^2 = \frac{2M}{\hbar^2}$. Let $v(x) \in C^2[a,b]$ be a nonzero function. Let $\gamma(x) \in C^2[a,b]$ be strictly increasing, such that $\gamma(a) = \alpha$ and $\gamma(b) = \beta$. Now we can define $w(\gamma(x))$ such that $\lambda(\hbar;x) = v(x)w(\gamma(x))$. Inserting this "ansatz" into the Schrödinger equation we get

$$w''(\gamma(x))v(x)\gamma'(x) + w'(\gamma(x))\{2v'(x)\gamma'(x) + v(x)\gamma''(x)\} \quad (2.5)$$
$$+w(\gamma(x))\{v''(x) + \rho^2 Q(x,E)v(x)\} = 0.$$

We let $v(x) = Q(x,E)^{-1/4}$ and $\gamma(x) = \int_{x_0}^{x}\sqrt{Q(y,E)}dy$ where $x_0 \in [a,b]$ is arbitrary. We do a change of variables from x to γ, noting that

$$\frac{d}{dx} = \sqrt{Q(\gamma,E)}\frac{d}{d\gamma}$$
$$\frac{d^2}{dx^2} = \sqrt{Q(\gamma,E)}\left(\frac{d}{d\gamma}\sqrt{Q(\gamma,E)}\frac{d}{d\gamma}\right).$$

Equation (2.2.5) is now reduced to

$$w''(\gamma) + w(\gamma)\left\{\frac{3}{16}\frac{Q'(\gamma,E)^2}{Q(\gamma,E)^2} - \frac{1}{4}\frac{Q''(\gamma,E)}{Q(\gamma,E)} + \rho^2\right\} = 0 \quad (2.6)$$
$$w''(\gamma) + w(\gamma)\left\{r(\gamma) + \rho^2\right\} = 0. \quad (2.7)$$

The choice of $r(\gamma)$ is obvious. Let

$$u_1(\gamma) = e^{i\rho\gamma}$$
$$u_2(\gamma) = e^{-i\rho\gamma}.$$

Using a variation of parameters type argument, the general solution to (2.7) can be given by

$$w(\gamma) = c_1u_1(\gamma) + c_2u_2(\gamma) + \frac{i}{2\rho}\int_{\alpha}^{\gamma}\left[u_1(\gamma)u_2(\xi) - u_2(\gamma)u_1(\xi)\right]r(\xi)w(\xi)d\xi \quad (2.8)$$

or

$$w(\gamma) = c_1u_1(\gamma) + c_2u_2(\gamma) - \frac{i}{2\rho}\int_{\gamma}^{\beta}\left[u_1(\gamma)u_2(\xi) - u_2(\gamma)u_1(\xi)\right]r(\xi)w(\xi)d\xi. \quad (2.9)$$

Without loss of generality consider the solution $w_1(\gamma)$ to (2.8) with $c_1 = 1, c_2 = 0$. Letting $h(\gamma) = \frac{w_1(\gamma)}{u_1(\gamma)}$ we have

$$h(\gamma) = 1 + \frac{i}{2\rho}\int_{\alpha}^{\gamma}\left[1 - e^{-i2\rho(\gamma-\xi)}\right] r(\xi)h(\xi)d\xi. \tag{2.10}$$

Mimicking standard existence and uniqueness proofs for differential equations we construct a solution to (2.10) using Picard approximations. Let

$$h_0(\gamma) = 0 \tag{2.11}$$

$$h_k(\gamma) = 1 + \frac{i}{2\rho}\int_{\alpha}^{\gamma}\left[1 - e^{-i2\rho(\gamma-\xi)}\right] r(\xi)h_{k-1}(\xi)d\xi \text{ for } k \geq 1. \tag{2.12}$$

Noting that for $0 \leq |1 - e^{-i2\rho(\gamma-\xi)}| \leq 2$, we see that

$$\mathcal{M} = \frac{\left|r(\xi)(1 - e^{-i2\rho(\gamma-\xi)})\right|}{2} \leq \max_{\xi\in[\alpha,\gamma]} |r(\xi)|.$$

A straightforward induction shows that

$$|h_k(\gamma) - h_{k-1}(\gamma)| \leq \frac{\mathcal{M}^k(\gamma-\alpha)^k}{\rho^k k!}. \tag{2.13}$$

From this it can be seen that for sufficiently large ρ the series $\{h_k(\gamma)\}$ is Cauchy, and thus convergent. We can now define the solution $h(\gamma)$ by

$$h(\gamma) = \lim_{k\to\infty} h_k(\gamma), \tag{2.14}$$

$$= \sum_{j=0}^{\infty}\{h_{j+1}(\gamma) - h_j(\gamma)\}. \tag{2.15}$$

So now for sufficiently large ρ we have

$$|h(\gamma) - h_k(\gamma)| \leq \sum_{j=k}^{\infty}|h_{j+1}(\gamma) - h_j(\gamma)| \tag{2.16}$$

$$\leq \sum_{j=k}^{\infty}\frac{\mathcal{M}^j(\gamma-\alpha)^j}{\rho^j j!} \tag{2.17}$$

$$\leq \frac{\mathcal{M}^k(\xi-\alpha)^k}{\rho^k} \tag{2.18}$$

$$= O(\rho^{-k}). \tag{2.19}$$

Returning to the original Schrödinger equation we now have that our solution is given by

$$\begin{aligned}\lambda(\hbar;x) &= v(x)w(\gamma(x)) \\ &= v(x)u_1(\gamma(x))h(\gamma(x)) \\ &= v(x)u_1(\gamma(x))\{h_k(\gamma(x)) + O(\hbar^k)\}\end{aligned}$$

Making all the substitutions and letting $k = 1$ we get the theorem. □

Remark. In a similar manner one can construct a WKB approximation that solves the stationary Schrödinger equation in the classically forbidden region, $V(x) > E$, by

$$\begin{aligned}\lambda(\hbar;x) &= C_1(V(x)-E)^{-1/4}\exp\left\{\frac{\sqrt{2M}}{\hbar}\int_{x_0}^{x}\sqrt{V(y)-E}dy\right\}\{1+O(\hbar)\} \\ &+C_2(V(x)-E)^{-1/4}\exp\left\{\frac{-\sqrt{2M}}{\hbar}\int_{x_0}^{x}\sqrt{V(y)-E}dy\right\}\{1+O(\hbar)\}.\end{aligned} \tag{2.20}$$

Remark. We note that we can write the leading order term in (2.3) as

$$\lambda^{WKB}(\hbar;x) = \frac{A}{(E-V(x))^{1/4}}\sin\left\{\frac{\sqrt{2M}}{\hbar}\int_{x_1}^{x}\sqrt{(E-V(y))}dy + B\right\}. \tag{2.21}$$

where x_1 is a turning point of $V(x)$.

A difficulty in using the WKB approximation is the calculation of the normalization constants. We refer to [28] section III.1 to provide them.

Lemma 2.22. *Assume the hypothesis of Lemma 2.2. Assume further that the classically acceptable region is the region* (x_1, x_2) *and that* $V'(x_k) \neq 0$ *for* $j = 1, 2$. *Then constants* A *and* B *in expression (2.21) are*

$$A = \frac{2}{\sqrt{\triangle}}$$
$$B = \frac{\pi}{4}$$

where

$$\triangle = 2\int_{x_1}^{x_2}\frac{dx}{\sqrt{(2M)(E-V(x))}}.$$

After a particular choice of phase we can write the WKB approximate wave function for the classically acceptable region as

$$\begin{aligned}\lambda^{WKB}(\hbar,x) &= \frac{1}{(E-V(x))^{1/4}}\Bigg\{D^{+}\exp\left\{i\frac{\sqrt{2M}}{\hbar}\int_{x_0}^{x}\sqrt{E-V(y)}dy\right\} \\ &\quad +D^{-}\exp\left\{-i\frac{\sqrt{2M}}{\hbar}\int_{x_0}^{x}\sqrt{E-V(y)}dy\right\}\Bigg\},\end{aligned} \tag{2.23}$$

with

$$\begin{aligned}D^{+} &= \frac{A}{2}\exp\left\{i\frac{\sqrt{2M}}{\hbar}\int_{x_1}^{x_0}\sqrt{E-V(y)}dy - i\frac{\pi}{4}\right\}, \\ D^{-} &= \frac{A}{2}\exp\left\{-i\frac{\sqrt{2M}}{\hbar}\int_{x_1}^{x_0}\sqrt{E-V(y)}dy + i\frac{\pi}{4}\right\}.\end{aligned} \tag{2.24}$$

2.3 Localization of Energy Eigenvectors and Semiclassical Analysis of Low-Lying eigenstates

The WKB approximation suggests that the eigenfunctions should exhibit exponential decay outside of the classically allowable region. Our next step is to provide rigorous results in this direction. The first result has existed in the literature for quite some time. Here we provide a version of this result keeping track of the $\hbar$ dependence.

Lemma 2.25. *Let* $H(\hbar) = -\frac{\hbar^2}{2m}\triangle_x + V(x)$ *be a two body system. Suppose* $V \in C(\mathbb{R})$, $\lim_{||x||\to\infty} |V(x)| = 0$, *and*

$$H(\hbar)\lambda(\hbar,x) = E(\hbar)\lambda(\hbar)$$

with $E(\hbar) < 0$ *for all* $\hbar \geq 0$ *then*

$$\|\lambda(\hbar,x)\exp\{\delta|x|\}\|_2 < \infty$$

for $\delta < \frac{\sqrt{-2mE(\hbar)}}{\hbar}$.

Remark. In the literature one sees many different conditions on V for this result to be true. We choose the conditions from [17] since they are straightforward to state and fit our purposes.

Proof. This Lemma is essentially contained in the proof of Theorem C.3.5 of [30]. Let $U(\theta)\lambda(\hbar, x) = e^{i\theta x}\lambda(\hbar, x)$. $U(\theta)\lambda(\hbar, x)$ has an analytic continuation to $|\text{Im }\theta| < M$ if and only if $e^{\theta|x|}\lambda(\hbar, x) \in L^2$ for all $\theta < M$. It follows that for eigenfunctions $\lambda(\hbar, x)$ we need to show that $U(\theta)\lambda(\hbar, x)$ has a continuation to a neighborhood of $\mathbb{R}$ with

$$|\text{Im }\theta| < \frac{\sqrt{-2mE(\hbar)}}{\hbar}.$$

Define

$$H(\theta, \hbar) = e^{i\theta x}H(\hbar)e^{-i\theta x},$$

and then

$$H(\theta, \hbar) = H(\hbar) + \frac{\hbar^2}{2m}\theta^2 + \frac{\hbar^2 i\theta}{m}\frac{d}{dx}.$$

Following the proof in [30], if $H(\theta)$ has an analytic continuation to a neighborhood of $\mathbb{R}$, any discrete eigenvalue $E(\hbar)$ of $H(\hbar)$ will move analytically for θ near 0. If $\theta \in \mathbb{R}$ then $H(\theta, \hbar)$ is unitarily equivalent to $H(\hbar)$ and so $E(\theta, \hbar) = E(\hbar)$, since unitary equivalence implies that $\sigma_{disc}(H(\theta, \hbar)) = \sigma_{disc}(H(i\text{Im }\theta, \hbar))$. So long as an eigenvalue $E(\theta, \hbar)$ remains away from $\sigma_{ess}(H(\theta, \hbar))$ it is independent of θ. It can be seen that $E(\hbar) \notin \sigma_{ess}(H(\theta, \hbar))$ if $E(\hbar) < -\frac{\hbar^2}{2m}|Im\ \ \theta|^2$ proving the theorem. ☐

The next result is a main result of [2, 31].

Lemma 2.26. *Let Ω be some open interval in $\mathbb{R}$ and $V \in C^2$ a real potential bounded from below on Ω such that $V \in L^1_{loc}(\Omega)$. Let $H(\hbar)$ be the self adjoint realization of $-\frac{\hbar^2}{2}\triangle + V$ on $L^2(\Omega)$ with either Dirichlet or Neumann boundary condition on $\partial\Omega$. If V has a nondegenerate absolute minimum V_0 at x_0, then the nth eigenvalue $E_n(\hbar)$ of $H(\hbar)$ is $V_0 + (n + \frac{1}{2})V''(x_0)\hbar + O(\hbar^2)$ as $\hbar \to 0$.*

An analogous result holds for the eigenvectors as well. The difference between the ground state eigenvector and the ground state given by the Harmonic Oscillator approximation is $O(\hbar^{1/2})$ [2, 31].

2.4 Semiclassical Wave-Packets

Here we present the standard definition of the semiclassical wave-packets. The intuitive way we will think about a wave-packet is to note that a wave-packet is centered around the classical position a. The Fourier transform of the wave-packets is centered around the classical momentum η. These wave-packets also carry information about the uncertainty relation of quantum mechanics. Our construction is analogous to the standard construction of the harmonic oscillator eigenstates using raising and lowering operators. The details of the construction presented here can be found in [12]. Let $a, \eta \in \mathbb{R}^n$, and $\hbar > 0$. Furthermore assume that A and B are complex $n \times n$ matrices satisfying

$$A^t B - B^t A = 0 \tag{2.27}$$
$$A^* B + B^* A = 2I. \tag{2.28}$$

Conditions (2.27)-(2.28) are known to be equivalent to the following conditions.

- A and B are invertible;
- The real and imaginary parts of BA^{-1} are both real symmetric;
- Re BA^{-1} is strictly positive definite;
- (Re $BA^{-1})^{-1} = AA^*$.

Let $p = -i\hbar\nabla_x$ be the momentum operator. For any $v \in \mathbb{C}^n$ define associated raising and lowering operators by

$$\mathcal{A}(A, B, \hbar, a, \eta, v)^* = \frac{1}{\sqrt{2\hbar}}[\langle B\bar{v}, (x-a)\rangle - i\langle A\bar{v}, (p-\eta)\rangle]$$

and

$$\mathcal{A}(A, B, \hbar, a, \eta, v) = \frac{1}{\sqrt{2\hbar}}[\langle \bar{B}v, (x-a)\rangle + i\langle \bar{A}v, (p-\eta)\rangle].$$

Let $\{e_j\}$ be any orthonormal basis for $\mathbb{R}^n$, and define

$$\mathcal{A}_j(A, B, \hbar, a, \eta)^* = \mathcal{A}(A, B, \hbar, a, \eta, e_j)^*$$
$$\mathcal{A}_j(A, B, \hbar, a, \eta) = \mathcal{A}(A, B, \hbar, a, \eta, e_j).$$

Then define

$$\mathcal{A}(A, B, \hbar, a, \eta)^* = \frac{1}{\sqrt{2\hbar}}[B^*(x-a) - iA^*(p-\eta)]$$
$$\mathcal{A}(A, B, \hbar, a, \eta) = \frac{1}{\sqrt{2\hbar}}[B^t(x-a) + iA^t(p-\eta)],$$

where the representation is in terms of the above basis. Define $\phi_0(A, B, \hbar, a, \eta, \cdot)$ to be a normalized vector with respect to $L^2(\mathbb{R}^n)$ such that

$$\mathcal{A}(A, B, \hbar, a, \eta)\phi_0(A, B, \hbar, a, \eta, \cdot) = 0.$$

After a specific choice of phase we have

$$\phi_0(A, B, \hbar, a, \eta, x) = (\pi\hbar)^{\frac{-n}{4}}(\det(A))^{\frac{-1}{2}} \times \exp\{-\langle (x-a), BA^{-1}(x-a)\rangle/(2\hbar) + i\langle \eta, (x-a)\rangle/\hbar\}.$$

For any multi-index k, define

$$\phi_k(A,B,\hbar,a,\eta,x) = \frac{1}{\sqrt{k!}}(\mathcal{A}_1(A,B,\hbar,a,\eta)^*)^{k_1} \times \dots$$
$$\cdots \times (\mathcal{A}_n(A,B,\hbar,a,\eta)^*)^{k_n}\phi_0(A,B,\hbar,a,\eta,x).$$

Remark. The sign of $(\det(A))^{-1/2}$ is chosen to depend on initial conditions and continuity.

Remark. Given $A, B, \hbar, a, \eta$ fixed, the functions $\phi_k(A,B,\hbar,a,\eta,\cdot)$ form an orthonormal basis of $L^2(\mathbb{R}^n)$ [12].

Now we describe how to propagate a wave-packet semiclassically. Let $V^{(1)}(\cdot)$ denote $\vec{\nabla}V(\cdot)$, let $V^{(2)}(\cdot)$ denote the second derivative matrix of $V(\cdot)$. Let $S(t) \in \mathbb{R}$, $a(t), \eta(t) \in \mathbb{R}^n$, and $A(t), B(t) \in \mathbb{C}^{n\times n}$, all governed by the following system of ordinary differential equations:

$$\dot{a}(t) = \eta(t) \tag{2.29}$$
$$\dot{\eta}(t) = -V^{(1)}(a(t)) \tag{2.30}$$
$$\dot{A}(t) = iB(t) \tag{2.31}$$
$$\dot{B}(t) = iV^{(2)}(a(t))A(t) \tag{2.32}$$
$$\dot{S}(t) = \frac{(\eta(t))^2}{2} - V(a(t)). \tag{2.33}$$

Assume the initial conditions given such that $A(0), B(0)$ together satisfy (2.27)-(2.28) and $S(0) = 0$. It is known that $A(t), B(t)$ together still satisfy conditions (2.27)-(2.28) [12].

Remark. Let

$$W_{a(t)}(x) = V(a(t)) + \langle V^{(1)}(a(t)), (x-a(t))\rangle + \frac{1}{2}\langle (x-a(t)), V^{(2)}(a(t))(x-a(t))\rangle$$

The functions $\psi_k(x,t) = e^{iS(t)/\hbar}\phi_k(A(t),B(t),\hbar,a(t),\eta(t),x)$ provide exact solutions to the time dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi_k(x,t) = -\frac{\hbar^2}{2}\triangle_x\psi_k(x,t) + W_{a(t)}(x)\psi_k(x,t)$$
$$\psi_k(x,0) = \phi_k(A(0),B(0),\hbar,a(0),\eta(0),x).$$

The main theorem describing the difference between the semiclassical propagation and quantum propagation of each wave-packet for any finite time is stated and proven as Theorem 3.5 in [12].

Lemma 2.34. *Suppose $V \in C^3(\mathbb{R}^n)$ satisfies $-C_1 \leq V(x) \leq C_2 e^{Mx^2}$ for some C_1, C_2 and M. Let $(A(t), B(t), a(t), \eta(t), S(t))$ be a solution to the system (2.29)-(2.33) with appropriate initial conditions. Let $H(\hbar) = -\frac{\hbar^2}{2}\triangle + V(x)$. Then there exists some $C(k,t)$ such that*

$$\begin{aligned} &\|e^{-itH(\hbar)/\hbar}\phi_k(A(0), B(0), \hbar, a(0), \eta(0), x) \\ &\quad -e^{iS(t)/\hbar}\phi_k(A(t), B(t), \hbar, a(t), \eta(t), x)\| \leq C(k,t)\hbar^{1/2}. \end{aligned} \tag{2.35}$$

The scattering results presented in chapter 4 show that under appropriate decay conditions on $V(x)$, $C(0,t)$ can be taken to be constant in t. For details on how to construct higher order semiclassical approximations the reader is refered to [10]-[14].

For the majority of our study we only consider the propagation of the wave-packet

$$\phi_0(A(t), B(t), \hbar, a(t), \eta(t), x).$$

2.5 Quasiclassical quantization

In [15, 16] the wave-packet dynamics have been modified in order to obtain approximate eigenvalues and eigenfunctions when the corresponding classical mechanics has periodic orbits. These wave-packets are periodic in time and are related to quasimodes and quasienergies of the appropriate quantum Hamiltonian. The main difficulty in this case when constructing a time periodic wave-packet arises when considering the spreading variables $A(t), B(t)$. Under the dynamics generated by (2.32)-(2.33) these variables are not periodic except for specific Hamiltonians. The details of this section we have taken directly from [15] and more detail can be found there.

Let $H(\hbar) = -\frac{\hbar^2}{2}\frac{d^2}{dx^2} + V(x)$. We seek a quasienergy $E(\hbar) \in \mathbb{R}$ and a quasimode $\psi(\hbar, x) \in L^2(\mathbb{R}, dx)$ with $\|\psi(\hbar, \cdot)\|_2 = O(1)$ as $\hbar \to 0$ such that

$$\|\{H(\hbar) - E(\hbar)\}\psi(\hbar, \cdot)\|_2 \leq C\hbar^\lambda$$

for $\lambda > 1$. It is well known that this implies the existence of some spectrum in the interval $[E(\hbar) - C\hbar^\lambda, E(\hbar) + C\hbar^\lambda]$. In general the spacing between eigenvalues is on the order of $\hbar$, so the information given is not trivial.

Throughout this section assume

$$V \in C^5(\mathbb{R}), \tag{2.36}$$

$$V \text{ is bounded below by a constant,} \tag{2.37}$$

$$|V(x)| \leq Ce^{Mx^2} \text{ for some constants C and M,} \tag{2.38}$$

$$V_\pm = \lim_{x \to \pm\infty} V(x) \in \mathbb{R} \cup \{\infty\} \tag{2.39}$$

Define $E_{max} = \min\{V_-, V_+\}$. Throughout assume that $E < E_{max}$. Let $\gamma(E) = \{(q,p) \in \mathbb{R}^2 : H(q,p) = \frac{p^2}{2} + V(q) = E\}$. A trajectory γ is said to be **regular** if

$$q_- = \min\{q : (q,p) \in \gamma(E)\}$$
$$q_+ = \max\{q : (q,p) \in \gamma(E)\}$$

are distinct adjacent roots of $V(q) - E$ with $V'(q_-) < 0$ and $V'(q_+) > 0$. Under these conditions it is well known that the classical motion is periodic with minimal period $\tau(E)$. The period depends only on the energy so we can define

$$I(E) = \oint_{\gamma(E)} p dq,$$
$$\tau(E) = \frac{\partial}{\partial E} I(E),$$
$$f_E(H) = H + \frac{\tau'(E)}{2\tau(E)}(H - E)^2.$$

We now state the following result which is theorem 1 of [15].

Lemma 2.40. *Suppose V satisfies assumptions (2.36)-(2.39) and $E < E_{max}$. Suppose $\gamma(E)$ is a regular trajectory, and define $\alpha(E) = \frac{\tau'(E)}{2\tau(E)}$. Let A_0, and B_0 be complex numbers satisfying (2.27)-(2.28), $(a_0, \eta_0) \in \gamma(E)$, and let $a(t), \eta(t), A(t), B(t)$, and $S(t)$ be given by the unique solution of the system of ordinary differential equations*

$$\dot{a}(t) = \eta(t) \tag{2.41}$$
$$\dot{\eta}(t) = -V'(a(t)) \tag{2.42}$$
$$\dot{A}(t) = iB(t) + 2\alpha(E)\eta(t)(V'(a(t)) + i\eta(t)B(t)) \tag{2.43}$$
$$\dot{B}(t) = iV''(a(t))A(t) + 2i\alpha(E)V'(a(t))(V'(a(t))A(t) + i\eta(t)B(t)) \tag{2.44}$$
$$\dot{S}(t) = \frac{1}{2}\eta(t)^2 - V(a(t)) \tag{2.45}$$

subject to the initial conditions at $t = 0$ given by $(a_0, \eta_0, A_0, B_0, 0)$.
Then define

$$I(E) = E\tau(E) + S(\tau(E)). \tag{2.46}$$

We assume $\hbar$ and E satisfy the Bohr-Sommerfeld condition

$$I(E) = 2\pi\hbar n, \quad n \in \mathbb{Z}^+. \tag{2.47}$$

Now define

$$\psi_0^E(\hbar, x) = (\pi\hbar)^{-1/4}\sqrt{\frac{|\theta|}{2\tau(E)}} \int_0^{\tau(E)} e^{\frac{it}{\hbar}(E + \frac{\pi\hbar}{\tau(E)})} e^{iS(t)/\hbar} \phi_0(A(t), B(t), \hbar, a(t), \eta(t), x) dt,$$

where θ denotes the conserved quantity

$$\theta = V'(a(t))A(t) + i\eta(t)B(t).$$

As in section (2.4) the branch of the square root in the wave-packet is determined by continuity in t. Then there exists a constant C such that

$$\|\psi_0^E(\hbar,\cdot)\|_2 = 1 + O(\hbar^{1/2}) \tag{2.48}$$

$$\left\| \left\{ H(\hbar) - \left(E + \tfrac{\pi\hbar}{\tau(E)} \right) \right\} \psi_0^E(\hbar,\cdot) \right\| \leq C\hbar^{3/2} \|\psi_0^E(\hbar,\cdot)\|. \tag{2.49}$$

Remark. The equations (2.41)-(2.45) are the equations of motion for the classical system governed by the Hamiltonian $f_E(H)$. The solutions to (2.41)-(2.45) are all periodic with period $\tau(E)$.

Our main interest from this section will be in using the Bohr-Sommerfeld conditions to choose the approximate eigenvalues for the system. For our analysis we will use standard WKB to approximate the eigenfunctions. Note that given the quasistate E_q, x, such that $E_q - V(x) = O(1)$, and an actual eigenvalue, E_a satisfying $|E_a - E_q| = O(\hbar^\lambda)$, then we have

$$(E_a - V(x))^{-1/4} = (E_q - V(x))^{-1/4} + O(\hbar^\lambda). \tag{2.50}$$

Therefore the WKB approximation given in section (2.2) will still be within $O(\hbar)$ of the exact eigenfunction if we substitute E_q for E_a.

2.6 Appendix to chapter 2: Energy of a Wavepacket centered at a minimum.

Let $\phi_0(A, B, \hbar, a, \eta, x)$ be defined as in section 2.4. Define

$$E_c = \frac{\eta^2}{2m} + V(a).$$

We assume that $V \in C_0^2(\mathbb{R})$. The expectation value of Energy of ϕ_0 is defined to be

$$\mu_{H_{\phi_0}} = \langle \phi_0(A, B, \hbar, a, \eta, x), H\phi_0(A, B, \hbar, a, \eta, x) \rangle.$$

The mean value is now given by

$$\begin{aligned} \mu_{H_{\phi_0}} &= \left\langle \phi_0(A, B, \hbar, a, \eta, x), \left\{ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(a) \right\} \phi_0(A, B, \hbar, a, \eta, x) \right\rangle \\ &\quad + \left\langle \phi_0(A, B, \hbar, a, \eta, x), \{V(x) - V(a)\}\phi_0(A, B, \hbar, a, \eta, x) \right\rangle. \end{aligned}$$

By Taylor's theorem and since $V(x) \in C_0^2(\mathbb{R})$ we have

$$\begin{aligned}
& \left| \left\langle \phi_0(A,B,\hbar,a,\eta,x), \{V(x)-V(a)\}\phi_0(A,B,\hbar,a,\eta,x) \right\rangle \right| \\
\leq & \left| \left\langle \phi_0(A,B,\hbar,a,\eta,x), \left\{ V'(a)(x-a) + \frac{C}{2}(x-a)^2 \right\} \phi_0(A,B,\hbar,a,\eta,x) \right\rangle \right| \\
\leq & \; O(\hbar).
\end{aligned}$$

Now we have

$$\begin{aligned}
\mu_{H_{\phi_0}} &= E_c + \left\langle \phi_0(A,B,\hbar,a,\eta,x), \left\{ -\frac{\eta^2}{2m} - \frac{\hbar^2}{2m}\frac{d^2}{dx^2} \right\} \phi_0(A,B,\hbar,a,\eta,x) \right\rangle \\
&= E_c + \left\langle \phi_0(A,B,\hbar,a,\eta,x), \left\{ -\frac{\hbar B A^{-1}}{2m} + \frac{BA^{-1}(x-a)^2}{2m} \right.\right. \\
&\qquad \left.\left. - \frac{2iBA^{-1}(x-a)\eta}{2m} \right\} \phi_0(A,B,\hbar,a,\eta,x) \right\rangle \\
&= E_c + O(\hbar).
\end{aligned}$$

The energy variance of ϕ_0 about the expectation value is defined by

$$\begin{aligned}
\sigma^2_{E_{\phi_0}} &= \left\{ \|(H-E_c)\phi_0(A,B,\hbar,a,\eta)\|_2 + E_c - \mu_{H_{\phi_0}} \right\}^2 \\
&\leq \{ \|\{H-E_c\}\phi_0(A,B,\hbar,a,\eta,x)\|_2 + O(\hbar) \}^2 \\
&\leq \left\{ \left\| \left\{ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \frac{\eta^2}{2m} \right\} \phi_0(A,B,\hbar,a,\eta,x) \right\| + \| \{V(x)-V(a)\} \phi_0(A,B,\hbar,a,\eta,x) \| \right\}^2 + O(\hbar) \\
&= O(\hbar).
\end{aligned}$$

Chapter 3

The 2 body problem in Classical and Quantum Mechanics

3.1 Introduction to Scattering Theory

When discussing scattering, one discusses the dynamics of systems where essentially all of the states are asymptotically "free" in the limit $t \to \pm\infty$. More precisely, scattering theory concerns itself with the comparison of different dynamics for the same system of interacting particles, the interacting dynamics and a comparison free dynamics. In general the free dynamics is simpler than the interacting dynamics. In this chapter we will start by giving precise mathematical statements for some basic questions in scattering theory. Afterwards we will give a short discussion of two body scattering in classical and quantum mechanics.

3.2 Fundamental Notions of Scattering

Here we present some of the basic questions of scattering theory. Our discussion is taken primarily from section XI.1 from [25]. A more in-depth discussion of the fundamental notions of scattering theory can be found there. Let us begin by defining the notion of existence of the scattering states.

Let Σ denote the set of dynamical states, let $T_t, T_t^{(0)}$, denote the interacting and free dynamics respectively. Given $\rho \in \Sigma$ the state of the interacting system at time t is given by $T_t\rho$, likewise the state of the free system at time t is given by $T_t^{(0)}\rho$. The next notion we will discuss, namely **existence of scattering states** can be stated precisely as:
For any $\rho_\pm \in \Sigma$, there exists $\rho \in \Sigma$ such that

$$\lim_{t\to\pm\infty}(T_t\rho - T_t^{(0)}\rho_\pm) = 0.$$

The related concept of **uniqueness of scattering states** is stated precisely as given $\rho_\pm \in \Sigma$, there is no more than one ρ such that

$$\lim_{t\to\pm\infty}(T_t\rho - T_t^{(0)}\rho_\pm) = 0.$$

Existence and Uniqueness of scattering states provides for mappings between states at $t = \pm\infty$ and states defined at any finite time, often $t = 0$. The next notion, that of **weak asymptotic completeness** provides for a mapping between the states at $-\infty$ and the states at ∞. To state this explicitly we define the sets

$$\Sigma_{in} = \Sigma_- = \left\{\rho \in \Sigma : \text{ there exists } \rho_- \in \Sigma : \lim_{t\to-\infty}(T_t\rho - T_t^{(0)}\rho_-) = 0\right\}$$
$$\Sigma_{out} = \Sigma_+ = \left\{\rho \in \Sigma : \text{ there exists } \rho_+ \in \Sigma : \lim_{t\to\infty}(T_t\rho - T_t^{(0)}\rho_+) = 0\right\}.$$

Weak asymptotic completeness is now stated as $\Sigma_{in} = \Sigma_{out}$ modulo trivial sets. The meaning of these trivial sets varies depending on the setting we are working in. Once weak asymptotic completeness has been established, the bijections $\Omega^\pm$ can be defined on $\Sigma \to \Sigma_\pm$ such that for $\rho \in \Sigma$,

$$\lim_{t\to\pm\infty}(T_t(\Omega^\mp\rho) - T_t^{(0)}\rho) = 0.$$

The **scattering transformation** can now be defined as a mapping from $\Sigma \to \Sigma$, modulo trivial sets, to be

$$S = (\Omega^-)^{-1}\Omega^+.$$

The point is that if one considers a free state at $-\infty$ and acts on it with the scattering transformation one should get the correspononding free state at ∞. A related notion we wish to discuss is that of **asymptotic completeness**. One expects that every state should either be bound or free. For many systems there is an obvious definition for the set of bound states Σ_{bound} contained in Σ and disjoint from Σ_{out}. The usual expectation is stated as

$$\Sigma_{bound}\text{``}+\text{''}\Sigma_{in} = \Sigma = \Sigma_{bound}\text{``}+\text{''}\Sigma_{out}.$$

This "addition" is the appropriate set addition and depends on the dynamics that we are dealing with. For quantum mechanics this addition is the direct sum, while for classical mechanics this addition is the set union. Asymptotic completeness obviously implies weak asymptotic completeness.

3.3 Two Body Classical Scattering

The material from this section is taken primarily from section XI.2 of [25] which is itself based on [29]. Let us consider the dynamics generated by the potential $V(x)$. As discussed in section (1.1), the dynamics of this system in $\mathbb{R}^n$ is given by

$$\dot{q}(t) = p(t) \tag{3.1}$$
$$\dot{p}(t) = -\nabla V(q(t)), \tag{3.2}$$

where $q(t), p(t) \in \mathbb{R}^n$. We state the short-range hypothesis: $V(x)$ is a **short-range potential** provided that there exists constants $C_\alpha, \nu > 0$ such that

$$|(D^\alpha V)(x)| \leq C_{|\alpha|}(1 + |x|)^{-1-|\alpha|-\nu} \tag{3.3}$$

for $|\alpha| = 0, 1, 2, 3$. Now we state Theorem XI.1 of [25], the major existence and uniqueness result for two body classical scattering theory.

Theorem 3.4. Existence and Uniqueness of scattering states
Let $V(x) : \mathbb{R}^n \to \mathbb{R}$ be a short-range potential. Let $(q_-, p_-) \in \mathbb{R}^{2n}$ be given with $p_- \neq 0$. Then there exists a unique solution to equations (3.1)-(3.2) such that

$$\lim_{t \to -\infty} |p(t) - p_-| = 0 \tag{3.5}$$
$$\lim_{t \to -\infty} |q(t) - q_- - p_- t| = 0. \tag{3.6}$$

To discuss asymptotic completeness we need some preliminary definitions. Define $\Sigma_0 = \{(a + bt, b) : b \neq 0\}$. Define $(q^{\pm\infty}_{a,b}(t), p^{\pm\infty}_{a,b}(t))$ to be the solution of (3.1)-(3.2) that is asymptotic to an element of Σ_0 and define Σ_{in} and Σ_{out} in the obvious way. Define the wave operators $\Omega^\pm : \Sigma_0 \to \Sigma$ by

$$\Sigma^\pm(a, b) = (q^{\mp\infty}_{a,b}(0), p^{\mp\infty}_{a,b}(0)).$$

Of course it is possible for some orbits to be bounded. We thus define $\Sigma_{bound} = \Big\{ (q(t), p(t))$ governed by equations (3.1)-(3.2) such that $\sup_{t \in \mathbb{R}} |q(t)| < \infty \Big\}$.

Theorem 3.7. Asymptotic Completeness
Suppose $V(x)$ satisfies the short-range assumption. Then $\Sigma_{in}, \Sigma_{out}$ and $\Sigma \backslash \Sigma_{bound}$ agree up to sets of measure zero.

This is theorem XI.3 of [25]. With the concept of asymptotic completeness we can now define the S-transformation by

$$Sw = (\Omega^-)^{-1}(\Omega^+ w).$$

3.4 Scattering in Hilbert Space and two body scattering in Quantum Mechanics

In this section we start by describing scattering theory in a Hilbert Space $\mathcal{H}$. We use two body quantum scattering to illustrate the ideas. We consider two unitary groups e^{-iAt} and e^{-iBt} which are thought of as an interacting dynamics and free dynamics respectively. The statement "$e^{-iAt}\phi$ is asymptotically free as $t \to -\infty$" is rigorously stated as:

Given $\phi \in \mathcal{H}$ there exists a vector $\phi_- \in \mathcal{H}$ such that

$$\lim_{t\to-\infty} \left\| e^{-iBt}\phi_- - e^{-iAt}\phi \right\| = 0. \tag{3.8}$$

This brings us to the definition of wave operators: Let A and B be self-adjoint operators on $\mathcal{H}$ and let $P_{ac}(B)$ be the projection onto the absolutely continuous subspace of B. The **wave-operators** $\Omega^{\pm}(A, B)$ exist if the strong operator limits

$$\Omega^{\pm}(A, B) = s - \lim_{t\to\mp\infty} e^{iAt}e^{-iBt}P_{ac}(B) \tag{3.9}$$

exist. When $\Omega^{\pm}$ exist we define the sets $\mathcal{H}_+ =$ Ran Ω^+ and $\mathcal{H}_- =$ Ran Ω^-. The notion of **weak asymptotic completeness** is stated as $\mathcal{H}_+ = \mathcal{H}_-$, whereas **asymptotic completeness** is stated as $\mathcal{H}_+ = \mathcal{H}_- = [P_{pp}(A)\mathcal{H}]^{\perp}$. There exists an intermediate notion that we define here. Suppose that $\Omega^{\pm}(A, B)$ exist, the wave operators are **complete** if and only if

$$\mathcal{H}_+ = \mathcal{H}_- = \text{Ran } P_{ac}(A)$$

and so the asymptotic completeness is now equivalent to the statement $\Omega^{\pm}$ are complete and $\sigma_{sing}(A) = \varnothing$. Completeness can be reduced to a (still difficult) question about existence.

Lemma 3.10. *Suppose that both $\Omega^{\pm}(A, B)$ exist then they are complete if and only if $\Omega^{\pm}(B, A)$ exist.*

We warn the reader that in practice proving existence of the wave operators $\Omega^{\pm}(B, A)$ is usually much more difficult than proving the existence of the wave-operators $\Omega^{\pm}(A, B)$. The reason for this difficulty is that the dynamics governed by B is much simpler than that governed by A. However once completeness is established, asymptotic compeleteness becomes a problem falling under spectral theory. Moreover, the spectral condition is known to be true for a large, physically interesting class of potentials.

The next theorem provides an explicit method for determining whether the wave-operators exist.

Theorem 3.11. *(Cook's Method) Let A and B be self-adjoint operators and suppose that there is a set $\mathcal{D} \subset D(B) \bigcap P_{ac}(B)\mathcal{H}$ which is dense in $P_{ac}(B)\mathcal{H}$ so that for any $\phi \in \mathcal{D}$ there* *is a T_0 satisfying*

$$\text{For } |t| > T_0, e^{-iBt}\phi \in D(A), \tag{3.12}$$

$$\int_{T_0}^{\infty} \left[\|(B-A)e^{-iBt}\phi\| + \|(B-A)e^{iBt}\| \right] dt < \infty, \tag{3.13}$$

then $\Omega^{\pm}(A,B)$ exist.

We now state and prove existence and uniqueness of wave-operators for two body scattering in quantum mechanics. The proof we give is the second proof from [25] section XI.4, this proof only applies for $n \geq 3$. We stress that there are proofs of this and similar statements that apply for $n \geq 1$ [20, 25], however many of the technical details are quite different. We present this proof in order to illustrate some of the complications arising when discussing scattering theory in low dimension.

Theorem 3.14. *(the Cook-Hack Theorem) Let $V \in L^2(\mathbb{R}^n) + L^r(\mathbb{R}^n)$ for $2 \leq r < n$. Let $H_0 = -\triangle$ on $L^2(\mathbb{R}^n)$ and let $H = H_0 + V$. Then $\Omega^{\pm}(H, H_0)$ exist.*

Proof for $n \geq 3$.
By Cook's method we need to show that given $\phi \in \mathcal{S}$, the Schwartz space, $\|Ve^{-itH_0}\phi\|_2 \in L^1(T_0, \infty)$ for some T_0. It is well known [24] that

$$\|e^{-itH_0}\phi\|_p \leq t^{-n\left(\frac{1}{2}-\frac{1}{p}\right)}\|\phi\|_q \tag{3.15}$$

where $\frac{1}{p} + \frac{1}{q} = 1$ and $2 \leq p \leq \infty$. We write $V = V_2 + V_r$ where in the obvious way $V_\alpha \in L^\alpha(\mathbb{R}^n)$. Let $\frac{1}{p} = \frac{1}{2} - \frac{1}{r}$ and so $\frac{1}{2} - \frac{1}{p} = \frac{1}{r} > \frac{1}{n}$. Now by Hölder's inequality we get that

$$\begin{aligned} \|Ve^{-itH_0}\|_2 &\leq \|V_2\|_2\|e^{-iH_0t}\phi\|_\infty + \|V_r\|_r\|e^{-iH_0t}\phi\|_p \\ &\leq \|V_2\|_2\|\phi\|_1 t^{-n/2} + \|V_r\|_r\|\phi\|_q t^{-n\left(\frac{1}{2}-\frac{1}{p}\right)}. \end{aligned} \tag{3.16}$$

Both terms in the above sum are in $L^1(T_0, \infty)$ for any $T_0 > 0$ completing the proof. □

This proof fails for integers $n < 3$ since $t^{-n/2} \notin L^1(\mathbb{R}^n)$ for $n \leq 2$. This phenomenon leads to added difficulty for scattering theory in low dimension when using arguments based on Cook's Method.

The question of asymptotic completeness for 2 and N-body problems was a central question driving research in scattering theory throughout much of the later half of the twentieth century. To begin we define some notions. Let A and B be densely defined linear operators on $\mathcal{H}$. Suppose that:

$$D(A) \subset D(B) \tag{3.17}$$

$$\exists a, b \in \mathbb{R} \text{ such that for all } \phi \in D(A) \tag{3.18}$$
$$\|B\phi\| \leq a\|A\phi\| + b\|\phi\|$$

B is said to be A-bounded. The relative bound of B with respect to A is defined to be the infinum of such a. An in depth discussion on when $H = -\triangle + V$ is $-\triangle$-bounded is in [24]. Now following [25] we define an **Enss potential** to be any symmetric operator V on $L^2(\mathbb{R}^n)$ such that

a) V is a relatively bounded pertubation of $H_0 = -\triangle$ with relative bound $a < 1$.
b) The function h on $[0, \infty)$ given by $h(R) = \|V(H_0 + i)^{-1}\chi(|x| \geq R)\|$ is in $L^1(0, \infty)$.

In the above $\chi(\cdot)$ is the characteristic function. We now state

Theorem 3.19. *(Enss's Theorem) Let V be an Enss potential and let $H = H_0 + V$ as a self-adjoint operator sum. Then*
1) The Wave Operators $\Omega^{\pm}(H, H_0)$ exist and are complete.
2) $\sigma_{sing}(H)$ is empty.
3) The only possible (finite) accumulation point for $\sigma_{pp}(H)$ is 0 and any nonzero eigenvalue has finite multiplicity.

This provides an answer to the question of Asymptotic Completeness since short range potentials as defined by (3.3) are contained in the set of Enss potentials.

Chapter 4

Scattering of Semiclassical Wavepackets

4.1 Introduction

Here we discuss scattering theory for the semiclassical wavepacket $\phi_0(A(t), B(t), \hbar, a(t), \eta(t), x)$ defined in section (2.4). The bulk of this chapter comes from the forthcoming paper [26]. Let

$$H(\hbar) = -\frac{\hbar^2}{2}\triangle_x + V(x),$$

and

$$H_1(t, \hbar) = -\frac{\hbar^2}{2}\triangle_x + W_{a(t)}(x),$$

with corresponding unitary propagators $U(t)$, and $U_1(t, 0)$ respectively. Recall that

$$U_1(t, 0)\phi_0(A(0), B(0), \hbar, a(0), \eta(0), x) = e^{iS(t)/\hbar}\phi_0(A(t), B(t), \hbar, a(t), \eta(t), x).$$

Now we present the main result of this chapter. Essentially the theorem shows that under sufficient decay conditions semiclassical scattering information can be extracted from a wavepacket in one and two dimensions. This result has been known for some time for dimension $n \geq 3$.

Theorem 4.1. *If V(x) satisfies the short range assumption (3.3), then there exists $C, \lambda > 0$, both independent of t and $\hbar$ such that*

$$\left\|U(t)\phi_0(A(0), B(0), \hbar, a(0), \eta(0), \cdot) - e^{iS(t)/\hbar}\phi_0(A(t), B(t), \hbar, a(t), \eta(t), \cdot)\right\|_2 \leq C\hbar^{\lambda}$$

for all $t \in (-\infty, \infty)$, $\hbar \in (0, 1)$, and any $A(0), B(0)$, satisfying equations (2.27)-(2.28) and almost all $a(0), \eta(0)$.

4.2 Classical Scattering

Existence of scattering states in classical mechanics is crucial to our study:

Lemma 4.2. *Let $V(x)$ satisfy the short range assumption. Let $(a_-, \eta_-) \in \mathbb{R}^{2n}$ such that $\eta_- \neq 0$. Let A_-, and B_- be complex $n \times n$ matrices satisfying conditions (2.27)-(2.28). There exists a unique solution*
$[a(t), \eta(t), A(t), B(t), S(t)]$ to the system (2.29)-(2.33) such that

$$\begin{aligned}
&\lim_{t\to-\infty} |a(t) - a_- - \eta_- t| = 0 \\
&\lim_{t\to-\infty} |\eta(t) - \eta_-| = 0 \\
&\lim_{t\to-\infty} |S(t) - t\eta_-^2/2| = 0 \\
&\lim_{t\to-\infty} \|A(t) - A_- - iB_- t\| = 0 \\
&\lim_{t\to-\infty} \|B(t) - B_-\| = 0
\end{aligned} \tag{4.3}$$

Moreover, there exist $n \times n$ complex matrices A_+, B_+ satisfying (2.27)-(2.28) and a closed set E of measure zero contained in $\mathbb{R}^{2n}$ such that $(a_-, \eta_-) \in \mathbb{R}^{2n} \backslash E$ implies the existence of $(a_+, \eta_+) \in \mathbb{R}^{2n}$ with $\eta_+ \neq 0$, $S_+ \in R$ such that

$$\begin{aligned}
&\lim_{t\to\infty} |a(t) - a_+ - \eta_+ t| = 0 \\
&\lim_{t\to\infty} |\eta(t) - \eta_+| = 0 \\
&\lim_{t\to\infty} \|A(t) - A_+ - iB_+ t\| = 0 \\
&\lim_{t\to\infty} \|B(t) - B_+\| = 0 \\
&\lim_{t\to\infty} |S(t) - S_+ - t\eta_+^2/2| = 0
\end{aligned} \tag{4.4}$$

This result basically says that given an incoming state, we can find an interacting state that approaches it at infinite negative time. Then for almost any free incoming state there exists a free outgoing state that approximates the interaction state at infinite time. This lemma is essentially Theorem (3.4) combined with Theorem (3.7). The details of the proof for the spreading variables $A(t), B(t)$ and the action variable $S(t)$, are given in [9].

4.3 Proof of Theorem 4.1 for n=1.

Theorem 4.1 was proven for $n \geq 3$ in [9]. The proof given there uses the fact that the wave-packet decays as $t^{-n/2}$, and thus the wave-packet is itself in L^1 for $n \geq 3$. For $n = 1$ and $n = 2$ we remove the portion of the state that has small asymptotic momentum. This portion of the wave-packet has norm $O(\hbar^{1/2})$. The remaining portion of the wave-packet decays fast enough in t to prove the estimates we need. The idea is to write the wave-packet as

$$\phi_0(A(t), B(t), \hbar, a(t), \eta(t), x) = \frac{p}{\eta}\phi_0(A(t), B(t), \hbar, a(t), \eta(t), x) + \frac{\eta - p}{\eta}\phi_0(A(t), B(t), \hbar, a(t), \eta(t), x).$$

and then drop the second term at time 0 in order to get the terms to cancel out correctly for large times. The intuition is that the second term above is on the order of $\sqrt{\hbar}$ at time zero and can be disregarded. The idea to write the wave-packet in this way was inspired by [20], and some technical details from this paper may be visible in the proof of the technical lemmas. Since we need the portion of the wave-packet kept to be propogated exactly by the semiclassics given in section (2.4), we write the wave-packet as

$$\begin{aligned} & \phi_0(A(\tau), B(\tau), \hbar, a(\tau), \eta(\tau), x) \\ = & \left\{1 + \frac{(x - a(\tau))iB_+}{A(\tau)\eta_+}\right\} \phi_0(A(\tau), B(\tau), \hbar, a(\tau), \eta(\tau), x) \\ & -\frac{(x - a(\tau))iB_+}{A(\tau)\eta_+}\phi_0(A(\tau), B(\tau), \hbar, a(\tau), \eta(\tau), x) \\ = & \left\{1 + \frac{(x - a(\tau))iB_+}{A(\tau)\eta_+}\right\} \phi_0(A(\tau), B(\tau), \hbar, a(\tau), \eta(\tau), x) \\ & -\sqrt{\frac{\hbar}{2}}\frac{iB_+}{\eta_+}\phi_1(A(\tau), B(\tau), \hbar, a(\tau), \eta(\tau), x). \\ = & \tilde{\phi}_0(A(\tau), B(\tau), \hbar, a(\tau), \eta(\tau), x) - \sqrt{\frac{\hbar}{2}}\frac{iB_+}{\eta_+}\phi_1(A(\tau), B(\tau), \hbar, a(\tau), \eta(\tau), x). \end{aligned} \tag{4.5}$$

We have used the fact that in one dimension

$$\phi_1(A(t), B(t), \hbar, a(t), \eta(t), x) = \sqrt{\frac{2}{\hbar}}\frac{(x - a(t))}{A(t)}\phi_0(A(t), B(t), \hbar, a(t), \eta(t), x). \tag{4.6}$$

Other than this separation of the wave-packet at $t = 0$ and Lemmas (4.11) and (4.12) the proof here essentially follows the proof for $n \geq 3$.
Proof of Theorem 4.1 for n=1.
Let $0 < \mu < 1, \epsilon \in (0, \frac{1}{6})$, and define

$$\chi_1(\hbar, a(t), x) = \begin{cases} 1 & \text{if } |x - a(t)| \leq (1 + |a(t)|)\mu\hbar^{1/2-\epsilon}, \\ 0 & \text{otherwise.} \end{cases}$$

Define $\chi_2(\hbar, a(t), x) = 1 - \chi_1(\hbar, a(t), x)$. Now define $\tilde{\phi}_0(A(\tau), B(\tau), \hbar, a(\tau), \eta(\tau), x)$ as above. We proceed to calculate. By (4.5) and the uniform boundedness of $\{U(t) - U_1(t,0)\}$ it is clear that

$$\begin{aligned} & \|\{U(t) - U_1(t,0)\}\, \phi_0(A(0), B(0), \hbar, a(0), \eta(0), \cdot)\|_2 \\ \leq & \left\|\{U(t) - U_1(t,0)\}\, \tilde{\phi}_0(A(0), B(0), \hbar, a(0), \eta(0), \cdot)\right\|_2 + k\sqrt{\hbar} \end{aligned}$$

Where

$$k = \frac{\sqrt{2}|B_+|}{|\eta_+|}.$$

By the fundamental theorem of calculus

$$\begin{aligned} & \left\|\{U(t) - U_1(t,0)\}\, \tilde{\phi}_0(A(0), B(0), \hbar, a(0), \eta(0), \cdot)\right\|_2 \\ = & \left\|\int_0^t \frac{d}{ds}\{U(s) - U_1(s,0)\}\, \tilde{\phi}_0(A(0), B(0), \hbar, a(0), \eta(0), \cdot) ds\right\|_2 \\ \leq & \hbar^{-1}\int_0^t \left\|\left\{V(\cdot) - W_{a(s)}(\cdot)\right\} \tilde{\phi}_0(A(s), B(s), \hbar, a(s), \eta(s), \cdot)\right\|_2 ds. \end{aligned} \tag{4.7}$$

Analyzing the integrand in the last expression

$$\begin{aligned} & \left\|\left\{V(x) - W_{a(s)}(x)\right\} \tilde{\phi}_0(A(s), B(s), \hbar, a(s), \eta(s), x)\right\|_2 \\ \leq & \left\|\left\{V(x) - W_{a(s)}(x)\right\} \chi_1(\hbar, a(s), x)\tilde{\phi}_0(A(s), B(s), \hbar, a(s), \eta(s), x)\right\|_2 \\ & + \left\|V(x)\chi_2(\hbar, a(s), x)\tilde{\phi}_0(A(s), B(s), \hbar, a(s), \eta(s), x)\right\|_2 \\ & + \left\|W_{a(s)}(x)\chi_2(\hbar, a(s), x)\tilde{\phi}_0(A(s), B(s), \hbar, a(s), \eta(s), x)\right\|_2 \\ = & I(s) + II(s) + III(s). \end{aligned} \tag{4.8}$$

If $|x - a(s)| \leq (1 + |a(s)|)\mu\hbar^{1/2-\epsilon}$ then following the analysis from [9] we let $z_* \in \mathcal{Z} = \{z = rx + (1-r)y\}$ such that $|z_*| \leq |z|$ for all $z \in \mathcal{Z}$. By the fundamental theorem of calculus and the triangle inequality it can be seen that

$$\begin{aligned} |V_2(x) - V_2(y)| & \leq C_3(1 + |z|)^{-4-\nu}|x - y| \\ & \leq C_3(1 + |y| - |y - z|)^{-4-\nu} \\ & \leq C_3[(1 - \mu)(1 + |y|)^{-4-\nu}|x - y|, \end{aligned} \tag{4.9}$$

where C_3 is taken from the short range assumption. From here it follows that

$$\left\|\chi_1(\hbar, a(s), x)(V(x) - W_{a(s)}(x))\right\|_\infty \leq C_3(1 + |a(s)|)^{-1-\nu}\hbar^{3/2-3\epsilon}. \tag{4.10}$$

Hence

$$I(s) \le C_3(1+|a(s)|)^{-1-\nu}\hbar^{3/2-3\epsilon}\left(1+k\sqrt{\frac{\hbar}{2}}\right).$$

Following the argument in [9] we find that due to continuity and asymptotics of the classical quantities $a(s), A(s)$

$$\begin{aligned} II(s) &\le \left\|\chi_2(\hbar, a(s), x)\exp\left\{\frac{-(x-a(s))^2}{4|A(s)|^2\hbar}\right\}\right\|_\infty \\ &\times\left\|\chi_2(\hbar, a(s), x)V(x)\left(1+\frac{(x-a(s))iB_+}{A(s)\eta_+}\right)(\pi\hbar)^{-1/4}(A(s))^{-1/2}\exp\left\{\frac{-(x-a(s))^2}{4|A(s)|^2\hbar}\right\}\right\|_2 \\ &\le \exp\{-C'\hbar^{-2\epsilon}\} \\ &\times\left\|\chi_2(\hbar, a(s), x)V(x)\left(1+\frac{(x-a(s))iB_+}{A(s)\eta_+}\right)(\pi\hbar)^{-1/4}(A(s))^{-1/2}\exp\left\{\frac{-(x-a(s))^2}{4|A(s)|^2\hbar}\right\}\right\|_2 \end{aligned}$$

where C' is some constant independent of s and $\hbar$. By lemma 4.11 and dividing by $A(s)\eta_+$ there exists C_V, T_1 such that for $s > T_1$

$$II(s) \le C_V\hbar^{-1/2-\nu/2}\exp\{-C'\hbar^{-2\epsilon}\}|s|^{-1-\nu/2}.$$

We can do the same analysis with $III(s)$ using lemma 4.12 to show that there exists T_2, C_W such that for $s > T_2$

$$III(s) \le C_W\hbar^{-1}\exp\{-C'\hbar^{-2\epsilon}\}|s|^{-1-\nu}.$$

The Theorem is now proven by taking $T = max\,\{T_1, T_2\}$ and writing for $t > T$

$$\begin{aligned} &\hbar^{-1}\int_0^t (I(s)+II(s)+III(s))ds \\ = \;&\hbar^{-1}\left\{\int_0^T (I(s)+II(s)+III(s))ds + \int_T^t (I(s)+II(s)+III(s))ds\right\}. \end{aligned}$$

The first term is bounded by some $C_T\hbar^{1/2}$ by Lemma (2.34). The second term is bounded by some $C\hbar^{-2}\exp\{-C'\hbar^{-2\epsilon}\} + C_3\hbar^{1/2-3\epsilon}$ by the work shown here. In order to propagate to large negative times we write the modified wave-packet with η_-, B_- in place of η_+, B_+ and the details are the same. $\square$

4.4 Technical Lemmas

Lemma 4.11. *In space dimension one, if $V(x)$ satisfies the short range assumption (3.3), then there exists some constant C such that for t sufficiently large, $\hbar \in (0,1)$*

$$\left\| \chi_2(\hbar, a(t), x) V(x) \{\eta_+ A(t) + (x - a(t)) i B_+\} (\pi\hbar)^{-1/4} (A(t))^{-1/2} \exp\left\{ \frac{-(x-a(t))^2}{4|A(t)|^2 \hbar} \right\} \right\|_2 \leq C \hbar^{-1/2-\nu/2} t^{-\nu/2}$$

where $\chi_2(\hbar, a(t), x)$ is defined in the proof of theorem 4.1.

Proof. Let $k_1 > 0$. By Lemma (4.2) there exists T such that $t > T$ implies that

$$\begin{aligned} & \left\| \chi_2(\hbar, a(t), x) V(x) \{\eta_+ A(t) + (x - a(t)) i B_+\} (\pi\hbar)^{-1/4} (A(t))^{-1/2} \exp\left\{ \frac{-(x-a(t))^2}{4|A(t)|^2 \hbar} \right\} \right\|_2 \\ \leq & \left\| \chi_2(\hbar, a(t), x) V(x) \cdot \{\eta_+ (A_+ + i B_+ t) + (x - a_+ - \eta_+ t) i B_+\} \right. \\ & \left. \times (\pi\hbar)^{-1/4} (A(t))^{-1/2} \exp\left\{ \frac{-(x-a(t))^2}{4|A(t)|^2 \hbar} \right\} \right\|_2 \\ & + k_1 \hbar^{-1/4} |A(t)|^{-1/2}. \end{aligned}$$

Using the triangle inequality we find that

$$\begin{aligned} & \left\| \chi_2(\hbar, a(t), x) V(x) \cdot \{\eta_+ (A_+ + i B_+ t) + (x - a_+ - \eta_+ t) i B_+\} \right. \\ & \left. \times (\pi\hbar)^{-1/4} (A(t))^{-1/2} \exp\left\{ \frac{-(x-a(t))^2}{4|A(t)|^2 \hbar} \right\} \right\|_2 \\ \leq & \left\| V(x) \left[\eta_+ A_+\right] (\pi\hbar)^{-1/4} (A^{-1/2}(t)) \exp\left\{ \frac{-(x-a(t))^2}{4|A(t)|^2 \hbar} \right\} \right\|_2 \\ & + \left\| \chi_2(\hbar, a(t), x) V(x) \left[i B_+ (x - a_+)\right] (\pi\hbar)^{-1/4} (A^{-1/2}(t)) \exp\left\{ \frac{-(x-a(t))^2}{4|A(t)|^2 \hbar} \right\} \right\|_2. \end{aligned}$$

Since $V(x) \in L^2(\mathbb{R})$ we have some constant k_2 such that for large enough t

$$\left\| V(x) \left[\eta_+ A_+\right] (\pi\hbar)^{-1/4} (A^{-1/2}(t)) \exp\left\{ \frac{-(x-a(t))^2}{4|A(t)|^2 \hbar} \right\} \right\|_2 \leq k_2 \hbar^{-1/4} t^{-1/2}.$$

Similarly,

$$
\begin{aligned}
&\left\| \chi_2(\hbar, a(t), x) V(x) \left[i B_+ (x - a_+) \right] (\pi\hbar)^{-1/4} (A^{-1/2}(t)) \exp\left\{ \frac{-(x-a(t))^2}{4|A(t)|^2\hbar} \right\} \right\|_2 \\
\leq\ & \left\| i B_+ V(x) (x - a_+)^{1/2+\nu/2} \right\|_2 \\
&\times \left\| \chi_2(\hbar, a(t), x) (\pi\hbar)^{-1/4} (A(t))^{-1/2} (x - a_+)^{1/2-\nu/2} \exp\left\{ \frac{-(x-a(t))^2}{4|A(t)|^2\hbar} \right\} \right\|_\infty .
\end{aligned}
$$

The first factor is a constant independent of t and $\hbar$ by the short-range assumption. Evaluating the second term further we see that

$$
\begin{aligned}
&\left\| \chi_2(\hbar, a(t), x) (\pi\hbar)^{-1/4} (A(t))^{-1/2} (x - a_+)^{1/2-\nu/2} \exp\left\{ \frac{-(x-a(t))^2}{4|A(t)|^2\hbar} \right\} \right\|_\infty \\
=\ & \left\| \chi_2(\hbar, a(t), x) \frac{(x-a_+)^{1/2-\nu/2}}{(x-a(t))^{1/2-\nu/2}} \frac{(x-a(t))^{1/2-\nu/2}}{(\pi\hbar)^{1/4}(A(t))^{1/2}} \exp\left\{ \frac{-(x-a(t))^2}{4|A(t)|^2\hbar} \right\} \right\|_\infty \\
\leq\ & \left\| \chi_2(\hbar, a(t), x) \frac{(x-a_+)^{1/2-\nu/2}}{(x-a(t))^{1/2-\nu/2}} \right\|_\infty \\
&\qquad \times \left\| \chi_2(\hbar, a(t), x) \frac{(x-a(t))^{1/2-\nu/2}}{(\pi\hbar)^{1/4}(A(t))^{1/2}} \exp\left\{ \frac{-(x-a(t))^2}{4|A(t)|^2\hbar} \right\} \right\|_\infty \\
\leq\ & \left\| \chi_2(\hbar, a(t), x) \frac{(x-a_+)^{1/2-\nu/2}}{(x-a(t))^{1/2-\nu/2}} \right\|_\infty \\
&\qquad \times \frac{\hbar^{-\nu/4+\epsilon\nu/2}}{(\mu(1+|a(t)|))^{\nu/2}} \left\| \frac{(x-a(t))^{1/2}}{(\pi\hbar)^{1/4}(A(t))^{1/2}} \exp\left\{ \frac{-(x-a(t))^2}{4|A(t)|^2\hbar} \right\} \right\|_\infty
\end{aligned}
$$

The second norm in the last expression is bounded by a constant since it is the norm of a bounded function of $\frac{x-a(t)}{\sqrt{\hbar}A(t)}$. For the first norm we see that

$$
\left\| \chi_2(\hbar, a(t), x) \frac{(x-a_+)^{1/2-\nu/2}}{(x-a(t))^{1/2-\nu/2}} \right\|_\infty \leq \max\left\{ 1, \left\| \chi_2(\hbar, a(t), x) \frac{(x-a_+)}{(x-a(t))} \right\|_\infty \right\}
$$

Now we see that

$$
\begin{aligned}
&\left\| \chi_2(\hbar, a(t), x) \frac{(x-a_+)}{(x-a(t))} \right\|_\infty \\
\leq\ & \left\| \chi_2(\hbar, a(t), x) \frac{(x-a(t)+a(t)-a_+)}{(x-a(t))} \right\|_\infty \\
\leq\ & 1 + \left\| \chi_2(\hbar, a(t), x) \frac{(a(t)-a_+)}{(x-a(t))} \right\|_\infty
\end{aligned}
$$

$$
\begin{aligned}
&\le\ 1+\left\|\chi_2(\hbar,a(t),x)\frac{(a(t)-a_+)}{(1+a(t))\mu\hbar^{1/2-\nu/2)}}\right\|_\infty \\
&\le\ 1+k_3\hbar^{-1/2+\nu/2}.
\end{aligned}
$$

k_3 is a constant independent of t and $\hbar$. The Lemma now follows. □

Lemma 4.12. *If $V(x)$ satisfies the short range assumption (3.3), then there exists some constant C such that for large enough t, and $\hbar \in (0,1)$*

$$
\left\|W_{a(t)}(x)\left[1+\frac{(x-a(t))iB_+}{A(t)\eta_+}\right](\pi\hbar)^{-1/4}(A^{-1/2}(t))\exp\left\{\frac{-(x-a(t)^2}{4|A(t)|^2\hbar}\right\}\right\|_2 \le C\hbar^{-1}t^{-1-\nu}.
$$

Proof. Since $V(x)$ satisfies the short range condition there exists C_j $j=0,1,2$ such that

$$
\begin{aligned}
&\left\|W_{a(t)}(x)\left[1+\frac{(x-a(t))iB_+}{A(t)\eta_+}\right](\pi\hbar)^{-1/4}(A^{-1/2}(t))\exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_2 \\
\le\ &\sum_{j=0}^{2}C_j(1+|a(t)|)^{-1-j-\nu}\cdot|A(t)|^j\cdot 2^j\cdot\hbar^{\frac{j}{2}} \\
\times&\left\|\left(\frac{(x-a(t))}{2|A(t)|\hbar^{\frac{1}{2}}}\right)^j\cdot\left\{1+\frac{(x-a(t))iB_+}{A(t)\eta_+}\right\}(\pi\hbar)^{-1/4}(A(t))^{-1/2}\exp\left\{\frac{-(x-a(t))^2}{4|A(t)|^2\hbar}\right\}\right\|_2.
\end{aligned}
$$

A quick calculation shows that the norms in the last expression are bounded by constants independent of t and $\hbar$. □

4.5 Extension to 2 dimensions

The extension of this result to 2 dimensions is not quite straightforward due to the structure of higher order states in more than one dimension. Here we point out the changes that need to be made in the proof of Theorem 4.1 we have given in order to extend it to $n=2$. The techniques follow the construction given in [11]. We present this in a less general manner for the sake of clarity. Let $\{e_1,e_2\}$ be the standard basis for $\mathbb{R}^2$. By the polar decomposition theorem there exists a unique unitary matrix $U_A(t)$ such that $A(t)=|A(t)|U_A(t)$. We then define

$$
\tilde{H}_1(v,x)=2\langle v,x\rangle,
$$

and

$$
H_{e_j}(A(t);x)=\tilde{H}_1(U_A(t)e_j,x).
$$

Now we proceed to define the higher order wave-packet

$$\begin{aligned}\phi_{e_j}(A(t),B(t),\hbar,a(t),\eta(t),x) &= 2^{-1/2}H_{e_j}\left(A(t);\hbar^{-1/2}|A(t)|^{-1}(x-a(t))\right)\\ &\quad\times\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x)\\ &= 2^{1/2}\langle U_A(t)e_j,\hbar^{-1/2}|A(t)|^{-1}(x-a(t))\rangle\\ &\quad\times\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x)\end{aligned}$$

Now define

$$\begin{aligned}&\tilde{\phi}_0(A(t),B(t),\hbar,a(t),\eta(t),x)\\ &=\left\{1+\left\langle U_A(t)e_1,\frac{i|A(t)|^{-1}B_+(x-a(t))}{\langle e_1,\eta_+\rangle}\right\rangle\right\}\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x)\end{aligned}$$

and the modified wave-packet is again propagated exactly by semiclassics as in theorem 4.1. If $\langle e_1,\eta_+\rangle=0$ we can use $\langle e_1,\eta_+\rangle=0$, since classical scattering requires that $\eta_+\neq 0$. Recall

$$U_A(t) = |A(t)|^{-1}A(t),$$

implying

$$U_A^*(t)=A^{-1}(t)|A(t)|,$$

and so similar to the analysis in one dimension we have

$$\begin{aligned}&\tilde{\phi}_0(A(t),B(t),\hbar,a(t),\eta(t),x)\\ &=\left\{\frac{\langle e_1,\eta_+\rangle}{\langle e_1,\eta_+\rangle}+\left\langle e_1,\frac{iA^{-1}(t)B_+(x-a(t))}{\langle e_1,\eta_+\rangle}\right\rangle\right\}\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x)\\ &=\frac{1}{\langle e_1,\eta_+\rangle}\left\langle e_1,\eta_++A^{-1}(t)(x-a(t))iB_+\right\rangle\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x)\\ &=\frac{1}{\langle e_1,\eta_+\rangle}\left\langle e_1,A^{-1}(t)\left\{A(t)\eta_++(x-a(t))iB_+\right\}\right\rangle\phi_0(A(t),B(t),\hbar,a(t),\eta(t),x).\end{aligned}$$

Noting that the short-range assumption (3.3) implies

$$V(x)(1+x)^{\frac{\nu}{2}}\in L^2(\mathbb{R}^2)$$

and thus

$$\left\|iB_+V(x)(x-a_+)^{\nu/2}\right\|_2$$

is constant in place of

$$\left\|iB_+V(x)(x-a_+)^{1/2+\nu/2}\right\|_2$$

in the one dimensional case. With these changes the proof is now analogous to the proof for $n=1$.

Chapter 5

The N-Body Problem in Classical and Quantum Mechanics: $N \geq 3$.

5.1 Introduction

Several aspects of the $N-$body problem can be studied using scattering theory. Several complications arise when describing this problem. For the $N-$body problem the possibility of multi-body bound states arises. In this chapter we provide notation that makes it easier to discuss the $N-$body problem. Then we discuss existence, uniqueness, and asymptotic completeness for both classical and quantum $N-$body scattering.

5.2 Basic Kinematic considerations of N-body scattering

Here we will discuss N-body Hamiltonians. We use the reference [3] as our starting point to discuss the kinematics although some elements are different. A system of $N-$particles in $\mathbb{R}^d$ with pairwise interactions is governed by the Hamiltonian

$$H = \sum_{k=1}^{N} \frac{p_k^2}{2m_k} + \sum_{j<k}^{N} V_{jk}(x_j - x_k) \tag{5.1}$$

$$H = \sum_{k=1}^{N} \frac{p_k^2}{2m_k} + V(x) \tag{5.2}$$

where we assume that $V_{jk}(r) \to 0$ as $|r| \to \infty$. For the three body problem let the particles be denoted by 1,2,3. The Hamiltonian for this problem is given by

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{p_3^2}{2m_3} + V_1(x_2 - x_3) + V_2(x_1 - x_3) + V_3(x_2 - x_1). \tag{5.3}$$

After removing the center of mass we describe the possible combinations of particles by a family of subspaces $S_{\mathcal{A}} = \{S_a : a \in \mathcal{A}\}$ each representing a possible combination of particles. $S_{\mathcal{A}}$ is closed under intersections and contains at least $S_a = \{0\}$ and $S_a = X$. For the one dimensional three body problem define $X = \{x \in \mathbb{R}^3 : m_1x_1 + m_2x_2 + m_3x_3 = 0\}$ we have $\mathcal{A} = \{0, 1, 2, 3, bound\}$ and the subspaces

$$S_0 := (1),(2),(3) := X \tag{5.4}$$

$$S_1 := (23),(1) := \{x \in \mathbb{R}^3 : x_2 - x_3 = 0\} \bigcap X \tag{5.5}$$

$$S_2 := (2),(13) := \{x \in \mathbb{R}^3 : x_1 - x_3 = 0\} \bigcap X \tag{5.6}$$

$$S_3 := (12)(3) := \{x \in \mathbb{R}^3 : x_1 - x_2 = 0\} \bigcap X \tag{5.7}$$

$$S_{bound} := (123) := \{x \in \mathbb{R}^3 : x_1 = x_2 = x_3 = 0\} \bigcap X. \tag{5.8}$$

For each of the subspaces $S_a \in S_{\mathcal{A}}$, define $S^a = S_a^{\perp}$. Also define $\#a$ ={The number of clusters in each subspace}, so for the example given

$$\#0 = 3$$
$$\#1 = \#2 = \#3 = 2$$
$$\#bound = 1.$$

It is clear that any $x \in X$ can be written as $x = s_a + s^a$ where $s_a \in S_a$ and $s^a \in S^a$. We can write $V(x) = V_a(s_a) + I_a(x)$ where $I_a(x) \to 0$ as $|s^a| \to \infty$. For example for the collinear three-body problem, looking at the cluster represented by S_1, we have

$$S_1 = span\{e_1, e_2 + e_3\} \bigcap X$$
$$S^1 = span\{e_2 - e_3\} \bigcap X$$
$$V^1(s^1) = V_1(x_2 - x_3),$$
$$I_1(x) = V_2(x_1 - x_3) + V_3(x_2 - x_1).$$

Now we can write

$$H = H_a + I_a(x),$$

where

$$H_a = \frac{(p^a)^2}{2\mu} + H^a,$$

and

$$H^a = \frac{(p_a)^2}{2M} + V^a(s^a).$$

H^a describes the interaction inside the clusters and H_a describes the dynamics between clusters. M and μ are the appropriate reduced masses.

5.3 Classical N-body scattering

The details and results of this section are taken primarily from [3]. The Hamiltonian for an $N-$body problem in 3 dimensions with equal masses interacting through pairwise potentials can be given by

$$H = \frac{\xi^2}{2} + \sum_{a \in \mathcal{A}: \# a = 2} V^a(x^a). \tag{5.9}$$

$\{S^a : a \in \mathcal{A}\}$ is a family of subspaces with the properties defined in the previous section. We say a solution $(q(t), p(t))$ to the equations of motion is an **a-solution** if and only if

$$\lim_{t \to \infty} t^{-1} q(t) \in S_a \backslash \bigcup_{S_b \not\supset S_a} S_b. \tag{5.10}$$

For large time an a-solution is affected mainly by the cluster Hamiltonian

$$\begin{aligned} H_a &= \frac{\xi_a^2}{2} + \frac{\xi^{a2}}{2} + \sum_{S^b \supset S^a} V^b(s^b) \\ &= \frac{\xi_a^2}{2} + H^a. \end{aligned} \tag{5.11}$$

Define the remaining part of the interaction to be $I_a = H - H_a$ as in section (5.2). According to this convention the motion inside the clusters is governed by the sup-a coordinates while the motion between the clusters is governed by the sub-a coordinates. We begin by stating the property that will ensure existence and uniqueness of the wave operators. We do this for the collinear three body problem specifically but the technical details still resemble those of [3]. We also note that we state and prove this theorem in a coordinate system where we have removed the center of mass. This reduces our problem to an equivalent problem with only two variables.

Lemma 5.12. Existence and Uniqueness of Wave-Operators *Let $V_j(\cdot) \in C_0^3(\mathbb{R})$,$j = 1,2,3$ be pairwise potentials. Let $M > 0$ be the appropriate reduced mass. Let $(\tilde{a}_x(t), \tilde{\eta}_x(t))$*

be a periodic solution to

$$\tilde{a}_x'(t) = \tilde{\eta}_x(t)/M$$
$$\tilde{\eta}_x'(t) = -V_1'(\tilde{a}_x(t))$$

such that $\frac{\tilde{\eta}_x^2(t)}{2M} + V_1(\tilde{a}_x(t)) = E < 0$*. Let* $\tilde{\eta}_{y-}, \tilde{a}_{y-}$ *be given such that*

$$\tilde{\eta}_{y-} \neq 0. \tag{5.13}$$

There exists a unique solution to

$$\begin{aligned}
a_x'(t) &= \eta_x(t)/M \\
\eta_x'(t) &= -V_1'(a_x(t)) - \frac{1}{2}V_2'(a_y(t) + a_x(t)/2) + \frac{1}{2}V_3'(a_y(t) - a_x(t)/2) \\
a_y'(t) &= \eta_y(t)/\mu \\
\eta_y'(t) &= -\left\{V_2'\left(a_y(t) + a_x(t)/2\right) + V_3'\left(a_y(t) - a_x(t)/2\right)\right\}
\end{aligned}$$

and $T < 0$ *such that for* $t < T$*,*

$$\lim_{t\to-\infty} |a_x(t) - \tilde{a}_x(t)| = 0 \tag{5.14}$$
$$\lim_{t\to-\infty} |\eta_x(t) - \tilde{\eta}_x(t)| = 0 \tag{5.15}$$
$$|a_y(t) - \tilde{a}_{y-} - \tilde{\eta}_{y-}t/\mu| = 0 \tag{5.16}$$
$$|\eta_y(t) - \tilde{\eta}_{y-}| = 0. \tag{5.17}$$

Proof. Define $\tilde{a}_y(t) = \tilde{a}_{y-} + t\tilde{\eta}_{y-}$. Let $m \geq \sqrt{2C}$ where $\|V_1'\|_\infty \leq C$. Define $u(t) = a(t) - \tilde{a}(t)$. Now define

$$\mathcal{U}_T = \{u(t) \in C(-\infty, T) : \lim_{t\to-\infty} e^{m|t|}|u(t)| = 0\}.$$

and consider the norm $\|u(t)\| = \sup_{t\in(-\infty,T)} e^{m|t|}|u(t)|$. Now define

$$\mathcal{U}_T^\gamma = \{u \in \mathcal{U}_T : \|u\| \leq \gamma\}.$$

It is clear that we can choose $T_1 < 0$ such that

$$\tau \leq T_1 \implies \begin{array}{l} V_2'(a_y(\tau) + a_x(\tau)/2) = 0 \\ V_3'(a_y(\tau) - a_x(\tau)/2) = 0. \end{array}$$

Define $(\mathcal{F}u)(t)$ by

$$(\mathcal{F}u)(t) = \int_{-\infty}^{t}\int_{-\infty}^{s} \left[\begin{array}{c} -\frac{1}{2}\left\{V_2'\left(a_y(\tau) + a_x(\tau)/2\right) - V_3'\left(a_y(\tau) - a_x(\tau)/2\right)\right\} \\ -\left\{V_2'\left(a_y(\tau) + a_x(\tau)/2\right) + V_3'\left(a_y(\tau) - a_x(\tau)/2\right)\right\} \end{array}\right] d\tau ds$$
$$+ \int_{-\infty}^{t}\int_{-\infty}^{s} \left[\begin{array}{c} -\left\{V_1'(a_x(\tau)) - V_1'(\tilde{a}_x(\tau))\right\} \\ 0 \end{array}\right] d\tau ds.$$

We will show that $\mathcal{F}$ is a contraction on $\mathcal{U}_T$ for some T. For $t < T_1$

$$\begin{aligned}
|(\mathcal{F}u)(t)| &\leq \int_{-\infty}^{t}\int_{-\infty}^{s} |V_1'(a_x(\tau)) - V_1'(\tilde{a}_x(\tau))| d\tau ds \\
&\leq \int_{-\infty}^{t}\int_{-\infty}^{s} 2C|u_x(\tau)| d\tau ds \\
&\leq \int_{-\infty}^{t}\int_{-\infty}^{s} 2Ce^{m\tau}e^{-m\tau}|u_x(\tau)| d\tau ds \\
&\leq \int_{-\infty}^{t}\int_{-\infty}^{s} 2Ce^{m\tau}\gamma d\tau ds \\
&\leq \frac{2C}{m^2}e^{-m|t|}\gamma \\
&\leq \gamma.
\end{aligned}$$

Therefore $(\mathcal{F}u)(t)$ maps $\mathcal{U}_T$ into itself for $T < T_1$. In a similar manner as we choose T_1 we choose $T_2 < 0$ such that for $t < T_2$

$$\begin{aligned}
& |(\mathcal{F}u_1)(t) - (\mathcal{F}u_2)(t)| \\
\leq & \int_{-\infty}^{t}\int_{-\infty}^{s} |V_1'(\tilde{a}_x(\tau) + u_{1x}(\tau)) - V_1'(\tilde{a}_x(\tau) + u_{2x}(\tau))| d\tau ds \\
\leq & \int_{-\infty}^{t}\int_{-\infty}^{s} 2Ce^{mt}e^{-mt}|u_{1x}(\tau) - u_{2x}(\tau)| d\tau ds \\
\leq & \int_{-\infty}^{t}\int_{-\infty}^{s} 2C\|u_1 - u_2\|e^{m\tau} d\tau ds \\
\leq & \frac{2C}{m^2}e^{-m|t|}\|u_1 - u_2\| \\
< & \|u_1 - u_2\|.
\end{aligned}$$

and thus $\mathcal{F}$ is a contraction and therefore has a fixed point. The proof for positive time is analogous.

□

The fact that the dynamics for the unbound particle actually leaves the interaction region accounts for equations (5.16)-(5.17) to hold. These equations would not hold if our pairwise potentials were not compactly supported. There exist more generalizations to this particular result. This result is sufficient for our purposes since our discussion later is limited to compactly supported pairwise potentials.

Next we briefly discuss the difficult problem of Asymptotic Completeness for the $N-$body problem. The result is theorem (3.4) of [3]. We state it here without proof.

Lemma 5.18. *Suppose that for every $b \in \mathcal{A}$, $\nabla^2 V^b(s^b)$ is bounded and for every $\theta > 0$ there exists σ such that $|\nabla V^a(s^a)| < \sigma e^{-\theta|s^a|}$, then the following statements are true.*
1) For any solution $(q_a(t), p_a(t))$ generated by H_a such that

$$\lim_{t\to\infty} t^{-1} q_a(t) \in S^a \setminus \bigcup_{S^b \not\supset S^a} S^b \tag{5.19}$$

there exists a unique solution $(q(t), p(t))$ of the motion generated by H such that for any $\theta > 0$

$$\lim_{t\to\infty} e^{\theta t}(q_a(t) - q(t)) = 0, \tag{5.20}$$

$$\lim_{t\to\infty} t(p_a(t) - p(t)) = 0. \tag{5.21}$$

2) For any solution $(q(t), p(t))$ generated by H such that

$$\lim_{t\to\infty} t^{-1} q(t) \in S^a \setminus \bigcup_{S^b \not\supset S^a} s^b \tag{5.22}$$

there exists a unique solution $(q_a(t), p_a(t))$ of the motion generated by H_a such that for any $\theta > 0$

$$\lim_{t\to\infty} e^{\theta t}(q_a(t) - q(t)) = 0, \tag{5.23}$$

$$\lim_{t\to\infty} t(p_a(t) - p(t)) = 0. \tag{5.24}$$

The shortcomings of this result provide a major obstacle to providing an interesting scattering theory for N-body systems in classical mechanics. In [18] it is alluded to that a result similar to Lemma 5.18 is known for the 3-body problem with short-range potentials. However the framework is much different from the one presented here, and the proof is for the case of compactly supported pairwise potentials.

Next we present some results that show that unless the system starts out in a three body bound state the system cannot asymptotically approach a three body bound state. Here we can assume that the potentials are short range. The presentation is based on that in [4] section 5.3.

Let $a \in \mathcal{A}$, we define $B^{a,+}$ to be the set of initial conditions $(q^a, p^a) \in S^a \times X^a$ such that $q^a(t)$ is bounded for $t > 0$. The set

$$\sigma^a := H^a(B^{a,+})$$

is called the set of trapping energy levels of H^a. Define

$$\tau^a := \bigcup_{S_b \not\supset S_a} \sigma^b.$$

We now get the main proposition

Theorem 5.25. *Assume that the pairwise potentials satisfy*

$$\lim_{|s^b|\to\infty}(1+(s^b)^2)|\nabla_{s^b}V^b(s^b)| = 0,$$

then

$$[\min_{a\neq 0}\inf V^a(s^a), 0] \subset \tau^0$$
$$[\inf V(x), \min_{a\neq 0}\inf V^a(s^a)] \subset \sigma^0.$$

This theorem is the classical equivalent of the HVZ theorem of quantum mechanics which will be described in section 5.4.

5.4 N-body scattering in quantum mechanics

In this section we quickly state without proof some results concerning $N-$body scattering in quantum mechanics. As before define the total Hamiltonian

$$H = \sum_{k=1}^{N} -\frac{\hbar^2}{2m_k}\triangle_k + \sum_{j<k} V_{jk}(x_j - x_j).$$

Let $S_{\mathcal{A}} : \mathcal{A} = \{a_1, a_2, ..a_k\}$ be a family of subspaces on $\mathbb{R}^{d\cdot N}$ as defined in section (5.2). For each cluster a, define the cluster Hamiltonian H_a as before define the cluster wave-operators by

$$\Omega_a^{\pm} = s - \lim_{t\to\mp\infty} e^{itH}e^{-itH_a}P^a \otimes I$$

where P^a is the projection onto the pure point spectrum of H^a. Now define

$$\mathcal{H}_a^{\pm} = \text{Ran } \Omega_a^{\pm}$$

and

$$\mathcal{H}^{\pm} = \sum_{a\in\mathcal{A}} \mathcal{H}_a^{\pm}$$

and in much the same vein now as two body scattering theory we have [7]:

Theorem 5.26. *Assume the pair potentials $V_{jk}(r)$ satisfy*

$$\|V_{jk}(r)(H_0+1)^{-1}P(|r|>R)\| \leq C\cdot R^{-\mu_1} \quad (5.27)$$
$$\|\nabla V_{jk}(r)(H_0+1)^{-1}P(|r|>R)\| \leq C\cdot R^{-(1+\mu_2)} \quad (5.28)$$

for $\mu_1 > 1, \mu_2 > 0$. *Then the wave operators exist, their ranges are mutually orthogonal, and satisfy*

$$\bigoplus_{a\geq 2} Ran\ \Omega_a^{\pm} \subset Ran\ (1 - P_{pp}(H)).$$

Suppose further that $V_{jk}(H_0+1)^{-1}$ *and* $\nabla V_{jk}(r)(H_0+1)^{-1}$ *are compact on* $L^2(S^a)$ *then*

$$\bigoplus_{a\geq 2} Ran\ \Omega_a^{\pm} = Ran\ (1 - P_{pp}(H)). \tag{5.29}$$

(5.29) is Asymptotic completeness for the $N-$body problem. Next we state the HVZ theorem [8]. This theorem states that the bottom of the essential spectrum of the Hamiltonian is equal to the lowest element of the spectra of the nontrivial cluster Hamiltonians.

Theorem 5.30. *Let* H *be an N-body Hamiltonian. Then*

$$\sigma_{ess}(H) = [\Sigma, \infty)$$

where $\Sigma := \min_{\#a>1} \Sigma_a$ *and* $\Sigma_a := \min(\sigma(H_a))$.

The numbers in $[\Sigma, 0)$ are sums of bound state energies in $\sigma_{pp}(H_a)$ and free energies in the other direction.

Chapter 6

Semiclassical Analysis of the Collinear Three body problem

6.1 Introduction

The three-body problem is a fundamental problem in both classical and quantum mechanics. We give a semiclassical analysis of the collinear three body problem with pairwise compactly supported interactions. For convenience we assume the particles all have mass equal to 1. The Hamiltonian for this problem is

$$H(\hbar) = -\frac{\hbar^2}{2}\{\triangle_{r_1} + \triangle_{r_2} + \triangle_{r_3}\} + V_1(r_3 - r_2) + V_2(r_3 - r_1) + V_3(r_2 - r_1),$$

where r_i is the position of the ith particle for $i = 1, 2, 3$. We assume that the $V_i \in C_0^3(\mathbb{R})$. Under assumptions given later we expect that the solutions exhibit separation as $t \to \pm\infty$ into states where two of the particles are bound and the other particle is asymptotically free. We will assume that the total energy of the system is negative so that we need not consider states where all three states are asymptotically free.

6.2 Jacobi Coordinates

In this section we transform the Hamiltonian using clustered Jacobi coordinates [25]. We need consider only two clusters, denoted as the “1” and “3” systems. The omitted “2” system is not needed since we have restricted the motion to be collinear and the ordering of the particles does not change under classical mechanics. In the “1” system particles 2 and 3 are bound. Let $x_1 = r_3 - r_2$, and $y_1 = -r_1 + (r_3 + r_2)/2$. Likewise we define the “3” coordinates where particles 1 and 2 are bound, as $x_3 = r_2 - r_1$ and $y_3 = r_3 - (r_2 + r_1)/2$. It is a quick matter to see that we can transform directly from the (x_1, y_1) coordinates to the (x_3, y_3) coordinates by the transformation

$$\begin{bmatrix} x_3 \\ y_3 \end{bmatrix} = \begin{bmatrix} -\frac{1}{2} & 1 \\ \frac{3}{4} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} \tag{6.1}$$

Let J_{13} denote the transformation matrix. We should point out that J_{13} is not a unitary matrix however $J = J^{-1}$. We can rewrite the Hamiltonian in the appropriate coordinates as

$$\begin{aligned} H(\hbar) &= -\frac{\hbar^2}{2m}\triangle_R - \frac{\hbar^2}{2M}\triangle_{x_1} - \frac{\hbar^2}{2\mu}\triangle_{y_1} + V_1(x_1) + V_2(y_1 + x_1/2) + V_3(y_1 - x_1/2) \\ H(\hbar) &= -\frac{\hbar^2}{2m}\triangle_R - \frac{\hbar^2}{2M}\triangle_{x_3} - \frac{\hbar^2}{2\mu}\triangle_{y_3} + V_1(y_3 - x_3/2) + V_2(y_3 + x_3/2) + V_3(x_3) \end{aligned}$$

where $M = 1/2, m = 3, \mu = 2/3$ and $R = (r_1 + r_2 + r_3)/m$. The R motion describes motion for the center of mass and does not figure into the interaction.

The above coordinate systems (x_k, y_k), are convenient for describing motion under the assumption that particle k is free and the other two particles are bound together.

6.3 Modified Semiclassics

The semiclassical wavepackets described in section (2.3) are not directly suitable for describing bound states that arise from periodic orbits [15, 16]. Here we give a modification that provides a semiclassical description when the classical system separates into a free motion in one direction and periodic motion in the other. We provide the analysis in the clustered Jacobi coordinates suppressing the subscript. Let $a_y(0), \eta_y(0), S_y(t) \in \mathbb{R}$ and $A_{yy}(0), B_{yy}(0) \in \mathbb{C}$ be such that

$$\bar{A}_{yy}(0)B_{yy}(0) + \bar{B}_{yy}(0)A_{yy}(0) = 2. \tag{6.2}$$

Suppose that $a_y(t), \eta_y(t), A_{yy}(t), B_{yy}(t), S_y(t))$ are propogated freely

$$\dot{a}_y(t) = \frac{\eta_y(t)}{\mu} \tag{6.3}$$

$$\dot{\eta}_y(t) = 0 \tag{6.4}$$

$$\dot{A}_{yy}(t) = \frac{iB_{yy}(t)}{\mu} \tag{6.5}$$

$$\dot{B}_{yy}(t) = 0 \tag{6.6}$$

$$\dot{S}_y(t) = \frac{(\eta_y(t))^2}{2\mu}. \tag{6.7}$$

Define the k-channel Hamiltonian, for k=1,2,3 to be

$$H_k(\hbar) = -\frac{\hbar^2}{2M}\triangle_x + V_k(x) - \frac{\hbar^2}{2\mu}\triangle_y. \tag{6.8}$$

Suppose that $E_j(\hbar) < 0$, and $\lambda_j(\hbar, x)$ are an eigenpair for

$$h_k(\hbar) = -\frac{\hbar^2}{2M}\triangle_x + V_k(x).$$

We define

$$\psi_{jl}(x, y, \hbar, t) = \exp\left\{\frac{i}{\hbar}(S_y(t) - tE_j(\hbar))\right\}\lambda_j(\hbar, x)\phi_l(A_{yy}(t), B_{yy}(t), \hbar, a_y(t), \eta_y, y). \tag{6.9}$$

A straightforward computation shows that

$$i\hbar\frac{d}{dt}\psi_{jl}(x, y, \hbar, t) = H_k(\hbar)\psi_{jl}(x, y, \hbar, t). \tag{6.10}$$

6.4 Classical mechanics of the system

In this section we provide information about the asymptotic behavior of the classical mechanics under the condition that the pairwise potentials are compactly supported. Suppressing the subscript the classical mechanics is governed by the following system of equations

$$\dot{a}_x(t) = \eta_x(t)/M \tag{6.11}$$

$$\dot{\eta}_x(t) = -V_1'(a_x(t)) - \frac{1}{2}V_2'(a_y(t) + a_x(t)/2) + \frac{1}{2}V_3'(a_y(t) - a_x(t)/2) \tag{6.12}$$

$$\dot{a}_y(t) = \eta_y(t)/\mu \tag{6.13}$$

$$\dot{\eta}_y(t) = -\left\{V_2'\left(a_y(t) + a_x(t)/2\right) + V_3'\left(a_y(t) - a_x(t)/2\right)\right\}. \tag{6.14}$$

We start by stating

Lemma 6.15. *Let $V_j(\cdot) \in C_0^3(\mathbb{R})$ for $j = 1, 2, 3$. Let $(\tilde{a}_{x1_{in}}(t), \tilde{\eta}_{x1_{in}}(t))$ be a periodic solution to*

$$\dot{\tilde{a}}_{x1_{in}}(t) = \tilde{\eta}_{x1_{in}}(t)/M$$
$$\dot{\tilde{\eta}}_{x1_{in}}(t) = -V_1'(\tilde{a}_{x1_{in}}(t))$$

such that $\frac{\left(\tilde{\eta}_{x1_{in}}(t)\right)^2}{2M} + V_1(\tilde{a}_{x1_{in}}(t)) = E_{in} < 0$. *Let $(\tilde{\eta}_{y1_{in}}, \tilde{a}_{y1_{in}})$ be given such that*

$$\tilde{\eta}_{y1_{in}} \neq 0$$
$$|\tilde{\eta}_{y1_{in}}| < \sqrt{-2\mu E_{in}}.$$

Define the total energy

$$E = E_{in} + \frac{\tilde{\eta}_{y_{in}}^2}{2\mu}.$$

There exists a unique solution to equations (6.11)-(6.14), and $T < 0$ such that

$$\lim_{t \to -\infty} |a_{x_1}(t) - \tilde{a}_{x_{1_{in}}}(t)| = 0$$
$$\lim_{t \to -\infty} |\eta_{x_1}(t) - \tilde{\eta}_{x_{1_{in}}}(t)| = 0$$

and for $t < T$

$$\begin{aligned} a_{y_1}(t) &= \tilde{a}_{y_{1_{in}}} + \tilde{\eta}_{y_{1_{in}}} t/\mu \\ \eta_y(t) &= \tilde{\eta}_{y_{1_{in}}}. \end{aligned}$$

We also note that energy is conserved, ie:

$$\frac{\eta_{y_1}^2(t)}{2\mu} + \frac{\eta_{x_1}^2(t)}{2M} + V_1(a_{x_1}(t)) + V_2(a_{y_1}(t) + a_{x_1}(t)/2) + V_3(a_{y_1}(t) - a_{x_1}(t)/2) = E.$$

Moreover for almost all $(\tilde{\eta}_{y_{1_{in}}}, \tilde{a}_{y_{1_{in}}})$ there exists a unique $(\tilde{a}_{y_{k_{out}}}, \tilde{\eta}_{y_{k_{out}}}) \in \mathbb{R}$, and a periodic solution $(\tilde{a}_{x_{k_{out}}}(t), \tilde{\eta}_{x_{k_{out}}}(t))$ of

$$\dot{\tilde{a}}_{x_{k_{out}}}(t) = \tilde{\eta}_{x_{k_{out}}}(t)/M$$
$$\dot{\tilde{\eta}}_{x_{k_{out}}}(t) = -V_k'(\tilde{a}_{x_{k_{out}}}(t))$$

such that if we define the quantity E_{out} by

$$\frac{\tilde{\eta}_{x_{k_{out}}}^2(t)}{2M} + V_k(\tilde{a}_{x_{k_{out}}}(t)) = E_{out},$$

then

$$\frac{\tilde{\eta}_{y_{k_{out}}}^2}{2\mu} + E_{out} = E.$$

There exists T_2 and for $k = 1$ a unique solution to (6.11)-(6.14) such that

$$\lim_{t \to \infty} |a_{x_k}(t) - \tilde{a}_{x_k}(t)| = 0$$
$$\lim_{t \to \infty} |\eta_{x_k}(t) - \tilde{\eta}_{x_k}(t)| = 0$$

and for $t > T_2$

$$\begin{aligned} a_{y_k}(t) &= \tilde{a}_{y_k} + \tilde{\eta}_{y_k} t/\mu \\ \eta_{y_k}(t) &= \tilde{\eta}_{y_k}. \end{aligned}$$

For $k = 3$, recombination, there exists a unique solution to analagous equations in the 3-channel such that the asymptotic conditions as $t \to \infty$ are met.

By theorem (5.25) three body bound states won't play a role in our analysis. Furthermore $E < 0$, so free particle scattering isn't possible for these initial conditions. This is a combination of Lemmas (5.12), and Lemma (5.18) for the classical mechanics. The E defined above is the **total classical energy** of the system. Now we define for the two body cluster (23), a **cluster time** T_1^- to be such that

$$V_1'(a_x(T_1^-)) = 0$$
$$V_1''(a_x(T_1^-)) > 0$$

and for all T such that $T \leq T_1^-$

$$V_2(a_y(T) + a_x(T)/2) = 0$$
$$V_3(a_y(T) - a_x(T)/2) = 0.$$

In a similar manner we define cluster times for the exit channel $T_k^+, k \in \{1, 3\}$, here the subscript k denotes that the classical equations cluster into the "k" channel. It is at these cluster times that we can change between the semiclassical description of section (2.3) and the semiclassical description of section (6.3).

6.5 Transitions between the different Semiclassical approximations

Our goal is to give an approximation for the Schrödinger equation where we can control the error terms for all times. The idea of our approximation is that for t before the negative cluster time the proper approximation is given by the modified wave-packets defined in section (6.3) for the 1-channel. For t inside some finite region (T_1^-, T_k^+) where T_1^+, T_k^+ are cluster times, we use the wave-packets from section (2.3) to give the appropriate quantum dynamics. For t after a positive cluster time the proper approximation is given by the modified wave-packets in the appropriate coordinates. For convenience we will assume that $V''(a_x(T_1^-)) = 1$. We also assume that the original bound pair (23) is in its ground state as $t \to -\infty$.

At a cluster time T_1^- we will transform from the modified wave-packet into the regular wave-packet and propogate semiclassically in the sense of section (2.3) until a positive cluster time T_k^+ occurs. $k = 1$ if the diatom (23) is still a diatom after the interaction, if $k = 3$ there is a rearrangement and we have the (12) particles bound as $t \to \infty$. In the case where there is a rearrangement, we can change to the 3-channel coordinates and describe the state in terms of the modified semiclassics in the 3-channel coordinates.

The way we treat the spreading changes at negative cluster time is as follows. Since $V''(a_x(T_1^-)) = 1$ we define $A_{xx}(T_1^-) = B_{xx}(T_1^-) = 1$ and let $A_{yy}(T_1^-), B_{yy}(T_1^-)$ be given by the appropriate free dynamics described in section (6.4). Now we can define the matrix

$$A(T_1^-) = \begin{bmatrix} A_{xx}(T_1^-) & 0 \\ 0 & A_{yy}(T_1^-) \end{bmatrix},$$

and the $B(T_1^-)$ matrix in the analogous way. Clearly conditions (2.27)-(2.28) hold. The classical action at T_1^- is given by

$$S(T_1^-) = \frac{T_1^- \eta_y^2}{2\mu} - T_1^- E_{in}.$$

Let

$$\omega_0(\hbar, x) = (\pi\hbar)^{-1/4} \exp\left\{-\frac{(x - a_x(T_1^-))^2}{2\hbar}\right\},$$

It is known [2, 31], that the first eigenstate $\lambda_0(\hbar, x)$ of $h_1(\hbar)$ is given by

$$\lambda_0(\hbar, x) = \omega_0(\hbar, x) + O(\hbar^{1/2}).$$

In light of this it is clear that

$$\begin{aligned} &\omega_0(\hbar, x)\phi_0(\hbar, T_1^-, y) = \phi_0(\hbar, T_1^-, x, y), \Rightarrow \\ &\left\|\lambda_0(\hbar, x)\phi_0(\hbar, T_1^-, y) - \phi_0(\hbar, T_1^-, x, y)\right\| = O(\hbar^{1/2}). \end{aligned} \tag{6.16}$$

We point out that $\phi_0(\hbar, T_1^-, y)$ is a one dimensional wave-packet whereas $\phi_0(\hbar, T_1^-, x, y)$ is a two dimensional wave-packet. So (6.16) says that the transition at T_1^- into the two dimensional wave-packet from the product of a one dimensional wave-packet and a bound state is accurate to order $\hbar^{1/2}$. We then propogate using the semiclassical description of (2.3). The initial conditions are

$$\begin{aligned} a(T_1^-) &= (a_x(T_1^-), a_y(T_1^-)) \\ \eta(T_1^-) &= (\eta_x(T_1^-)), \eta_y(T_1^-)), \end{aligned}$$

and $A(T_1^-), B(T_1^-), S(T_1^-)$ as given before.

Next we discuss the change of coordinate systems. The only case we need to concern ourselves with is the case where there is a rearrangement of the classical mechanics. Recall from section (6.2) that

$$\begin{aligned} x_3 &= -\frac{1}{2}x_1 + y_1 \\ y_3 &= \frac{3}{4}x_1 + \frac{1}{2}y_1. \end{aligned}$$

In this sense if we have the relative motion $a(T_3^+)$ given by the classical mechanics in the "1" coordinate system. The motion in the 3-coordinates is given by $J_{13}a$ where J_{13} is defined by (6.1) The transformation of $\eta(T_3^+)$, the components of momentum, from 1-coordinates to 3-coordinates is given by $\eta \to (J_{13}^*)\eta$. To transform the spreading matrices A and B from the 1-coordinates to the 3-coordinates we use the transformations $A \to J_{13}A$, and $B \to (J_{13}^*)B$. A simple calculation shows that conditions (2.27)-(2.28) are still satisfied. Furthermore it is clear that the classical energy is conserved under this transformation. Without loss of generality we assume that a recombination of the particles does not occur. Therefore as time goes to ∞ particles (23) will remain bound.

For interaction times we have a two dimensional wave packet in the cluster coordinates. As noted before we want to approximate the states that exhibit a clustering at infinite time by those states that are products of free wavepackets in the y direction and bound states in the x direction. For large positive times the solutions that exhibit clustering are of the form

$$\sum_{E_\alpha(\hbar)} e^{-itE_\alpha(\hbar)/\hbar}\tilde{\lambda}_\alpha(\hbar,x)e^{iS_y^\alpha(t)/\hbar}\Phi_0^\alpha(\mathcal{A}_{yy}(t),\mathcal{B}_{yy}(t),\hbar,a_y^{out_\alpha}(t),\eta_y^{out_\alpha}(t),y).$$

Where $E_\alpha(\hbar)$ and $\lambda_\alpha(\hbar,x)$ are an eigenpair for

$$h_1(\hbar) = -\frac{\hbar^2}{2M}\triangle_x + V_1(x)$$

and $\tilde{\lambda}_\alpha(\hbar,x)$ is $\lambda_\alpha(\hbar,x)$ multiplied by a phase factor. The modified semiclassical wavepacket for the transverse direction and the initial values of it's parameters $\mathcal{A}_{yy}(t),\mathcal{B}_{yy}(t),a_y^{out_\alpha}(t),\eta_y^{out_\alpha}(t)$ will be determined by the equation

$$\begin{aligned} &\Phi_0^\alpha(\mathcal{A}_{yy}(t),\mathcal{B}_{yy}(t),\hbar,a_y^{out_\alpha}(t),\eta_y^{out_\alpha}(t),y) \\ = \;& C_\alpha(\hbar,T_1^+)\times\phi_0(\mathcal{A}_{yy}(t),\mathcal{B}_{yy}(t),\hbar,a_y^{out_\alpha}(t),\eta_y^{out_\alpha}(t),y) \end{aligned} \tag{6.17}$$

where

$$C_\alpha(\hbar,T_1^+) = \left\|\Phi_0^\alpha(A_{yy}(T_1^+),B_{yy}(T_1^+),\hbar,a_y^{out_\alpha}(T_1^+),\eta_y^{out_\alpha}(T_1^+),y)\right\|_2$$

and

$$\begin{aligned} &\Phi_0^\alpha(A_{yy}(T_1^+),B_{yy}(T_1^+),\hbar,a_y^{out_\alpha}(T_1^+),\eta_y^{out_\alpha}(T_1^+),y) \\ &\quad = \left\langle\lambda_\alpha(\hbar,x),\phi_0(A(T_1^+),B(T_1^+),\hbar,a(t_1^+),\eta(T_1^+),x,y)\right\rangle. \end{aligned}$$

The parameters for Φ_0^α will be propogated freely. Furthermore $\mathcal{A}_{yy}(T_1^+)$ and $\mathcal{B}_{yy}(T_1^+)$ at the transition time will be chosen to satisfy condition (6.2). The motion is concentrated near the orbit given by classical mechanics. A complete discussion on how $C_\alpha(\hbar,T_1^+)$, $A_{yy}(T_1^+)$, and $B_{yy}(T_1^+)$ are determined will be given in section (6.7).

6.6 The approximation

At this point we can give the main results of this chapter. For finite times we use the regular semiclassical approximation which we know is valid. We need to handle infinite times in a special way. We begin with the analysis for times approaching $-\infty$.

Theorem 6.18. *Suppose the pairwise potentials are all compactly supported. Let $\psi_{00}(x, y, \hbar, t)$ be a two dimensional semiclassical state defined in the manner of section (6.3) with the diatom in it's ground state. There exists a cluster time T_1^- such that*

$$\lim_{\hbar \to 0} \|U(t)\phi_0(A(0), B(0), \hbar, a(0), \eta(0), x, y) - \psi_{00}(x, y, \hbar, t)\|_2 = 0$$

uniformly in t for $t < T_1^-$.

The ψ_{00} in the theorem are those wave-packets described by equation (6.9). We have restricted our initial states to be such that $j = l = 0$. The proof is simply putting together all the technical details of the next few sections.

Proof.

$$\begin{aligned}
& \|U(t)\phi_0(A(0), B(0), \hbar, a(0), \eta(0), x, y) - \psi_{00}(x, y, \hbar, t)\| \\
= & \|U(t - T_1^-)U(T_1^-)\phi_0(A(0), B(0), \hbar, a(0), \eta(0), x, y) - \psi_{00}(x, y, \hbar, t)\| \\
\leq & \Bigg\| U(t - T_1^-)U(T_1^-)\phi_0(A(0), B(0), \hbar, a(0), \eta(0), x, y) \qquad (6.19) \\
& \quad -U(t - T_1^-) \exp\left\{\frac{i}{\hbar}S(T_1^-)\right\} \phi_0(A(T_1^-), B(T_1^-), \hbar, a(T_1^-), \eta(T_1^-), x, y) \Bigg\| \\
& + \Bigg\| U(t - T_1^-) \exp\left\{\frac{i}{\hbar}S(T_1^-)\right\} \phi_0(A(T_1^-), B(T_1^-), \hbar, a(T_1^-), \eta(T_1^-), x, y) \qquad (6.20) \\
& \qquad -U(t - T_1^-)\psi_{00}(x, y, \hbar, T_1^-) \Bigg\| \\
& + \|U(t - T_1^-)\psi_{00}(x, y, \hbar, T_1^-) - \psi_{00}(x, y, \hbar, t)\|. \qquad (6.21)
\end{aligned}$$

Lemma (2.34) shows that (6.20) $\leq C(T_1^-)\hbar^{1/2}$, (6.16) shows that (6.21) $\leq C\hbar^{1/2}$, and Theorem (6.64) shows that there exists $\epsilon > 0$ such that

$$\begin{aligned}
(6.22) \quad \leq \quad & C \exp\left\{-\frac{C_1|T_1^-|}{\hbar}\right\} + \\
& C|T_1^-|^{-1/2}\hbar^{-5/4} \exp\left\{-C_1\hbar^{-2\epsilon}\right\}.
\end{aligned}$$

□

In much the same way we have the result for times approaching ∞

Theorem 6.22. *Suppose the pairwise potentials are compactly supported. Let $E_\alpha(\hbar), \lambda_\alpha(\hbar, x)$ be a set of eigenpairs for the sub-Hamiltonian*

$$h_1(\hbar) = -\frac{\hbar^2}{2M}\triangle_x + V_1(x).$$

There exists a cluster time $T_1^+ > 0$ such that

$$\lim_{\hbar \to 0}\Bigg\| U(t)\phi_0(A(0), B(0), \hbar, a(0), \eta(0), x, y) \\ - \sum_\alpha e^{i[S_y^\alpha(T_1^+) - T_1^+ E_\alpha(\hbar)]/\hbar}\tilde{\lambda}_\alpha(\hbar, x)\Phi_0(\mathcal{A}(t), \mathcal{B}(t), \hbar, a^{out_\alpha}(t), \eta^{out_\alpha}(t), y)\Bigg\| = 0$$

uniformly in t for $t > T_1^+$. Let E_c be the energy of the classical sub-Hamiltonian

$$\frac{\eta_x^2}{2M} + V_1(a_x(t))$$

where $a_x(t), \eta_x(t)$ are determined by Lemma (5.12). Define

$$\tilde{\lambda}_\alpha(\hbar, x) = e^{-iT_1^+[E_c - E_j(\hbar)]/\hbar}\lambda_\alpha(\hbar, x).$$

Φ_0 is determined by equation (6.17).

The proof of this theorem is similar to the proof for the negative time analog.

Proof.

$$\Bigg\| U(t)\phi_0(A(0), B(0), \hbar, a(0), \eta(0), x, y) \\ - \sum_\alpha e^{i[S_y(T_1^+) - T_1^+ E_\alpha(\hbar)]/\hbar}\lambda_\alpha(\hbar, x)\Phi_0(\mathcal{A}(t), \mathcal{B}(t), \hbar, a^{out_\alpha}(t), \eta^{out_\alpha}(t), y)\Bigg\|$$

$$= \Bigg\| U(t - T_1^+)U(T_1^+)\phi_0(A(0), B(0), \hbar, a(0), \eta(0), x, y) \\ - \sum_\alpha e^{i[S_y(T_1^+) - T_1^+ E_\alpha(\hbar)]/\hbar}\tilde{\lambda}_\alpha(\hbar, x)\Phi_0(\mathcal{A}(t), \mathcal{B}(t), \hbar, a^{out_\alpha}(t), \eta^{out_\alpha}(t), y)\Bigg\|$$

$$\leq \Bigg\| U(t - T_1^+)U(T_1^+)\phi_0(A(0), B(0), \hbar, a(0), \eta(0), x, y) \tag{6.23}$$

$$- U(t - T_1^+) \exp\left\{ \frac{i}{\hbar} S(T_1^+) \right\} \phi_0(A(T_1^+), B(T_1^+), \hbar, a(T_1^+), \eta(T_1^+), x, y) \Bigg\|$$

$$+ \Bigg\| U(t - T_1^+) \exp\left\{ \frac{i}{\hbar} S(T_1^+) \right\} \phi_0(A(T_1^+), B(T_1^+), \hbar, a(T_1^+), \eta(T_1^+), x, y) \tag{6.24}$$

$$- U(t - T_1^+) \sum_\alpha e^{i[S_y(T_1^+) - T_1^+ E_\alpha(\hbar)]/\hbar} \tilde{\lambda}_\alpha(\hbar, x) \Phi_0(\mathcal{A}(t), \mathcal{B}(t), \hbar, a^{out_\alpha}(t), \eta^{out_\alpha}(t), y) \Bigg\|$$

$$+ \Bigg\| U(t - T_1^+) \sum_\alpha \lambda_\alpha(\hbar, x) \Phi_0(\mathcal{A}(t), \mathcal{B}(t), \hbar, a^{out_\alpha}(t), \eta^{out_\alpha}(t), y) \tag{6.25}$$

$$- \sum_\alpha e^{i[S_y(T_1^+) - T_1^+ E_\alpha(\hbar)]/\hbar} \tilde{\lambda}_\alpha(\hbar, x) \Phi_0(\mathcal{A}(t), \mathcal{B}(t), \hbar, a^{out_\alpha}(t), \eta^{out_\alpha}(t), y) \Bigg\|$$

By Lemma (2.34), (6.24) $\leq C(T_1^+)\hbar^{1/2}$.
Theorem (6.58) implies that

$$(6.25) \leq C\hbar^\nu.$$

Theorem (6.64) together with an argument we use to interpret (6.49) will imply that

$$\begin{aligned} (6.26) \quad \leq \quad & C\hbar^{-1} \exp\left\{ -\frac{C_1 |T_1^+|}{\hbar} \right\} + \\ & C|T_1^+|^{-1/2} \hbar^{-9/4} \exp\left\{ -C_1 \hbar^{-2\epsilon} \right\}. \end{aligned}$$

for some $\epsilon > 0$. □

6.7 Projecting onto the bound state

In this section we provide the analysis involved when projecting the two dimensional wave-packet $\phi_0(A, B, \hbar, a, \eta, x, y)$ onto a bound state $\lambda_\alpha(\hbar, x)$ for the one dimensional subsytem

$$h_1(\hbar) = -\frac{\hbar^2}{2M} \triangle_x + V_1(x)$$

as is described at the end of section 6.5. We begin by defining some terms to be used. Let

$$\lambda_j^\pm(\hbar, x) = \frac{1}{(E_j(\hbar) - V_1(x))^{1/4}} \exp\left\{ \pm \frac{i\sqrt{2M}}{\hbar} \int_{a_x(T_1^+)}^x \sqrt{E_j(\hbar) - V_1(\xi)} d\xi \right\}$$

$$\theta_j^\pm(\hbar, x) = \frac{1}{(E_j(\hbar) - V_1(a_x(T_1^+)))^{1/4}} \exp\left\{ \pm \frac{i\sqrt{2M}}{\hbar} \sqrt{E_j(\hbar) - V_1(a_x(T_1^+))} (x - a_x(T_1^+)) \right\}.$$

We note here that if the quantum number j used to choose the orbit through Bohr-Sommerfeld quantization is greater than $C\hbar^{-1}$ then $|E_j(\hbar) - V_1(a_x(t))| = O(1)$. This is seen by recalling Lemma 2.26. Let us start this section by doing a computation.

Lemma 6.26. *For those cluster times T_1^+ such that $E_j(\hbar) - V_1(a_x(T_1^+)) > 0$*

$$\langle \theta_j^{\pm}(\hbar, x), \phi_0(T_1^+, \hbar, x, y)\rangle_{dx}$$

is a Semiclassical wave-packet in y.

Proof. Let $z = (x, y)$. To ease the notation we define the following

$$\begin{aligned} k &= \sqrt{(2M)(E_j(\hbar) - V_1(a_x(T_1^+)))} \\ F &= B(T_1^+)A^{-1}(T_1^+) \\ \xi^{\pm} &= \mp k\hat{e}_x + \eta(T_1^+) \end{aligned}$$

where we note that k is a scalar, F is a 2×2 matrix and $\xi^{\pm}$ is a 2 dimensional vector. Now the above inner product can be written as

$$\begin{aligned} &\frac{(\pi\hbar)^{-1/2}}{(E_j(\hbar) - V_1(a_x(T_1^+))^{1/4})(\det A(T_1^+))^{1/2}} \\ &\times \int_{\mathbb{R}} \exp\left\{\frac{i}{\hbar}\langle \xi^{\pm}, (z - a(T_1^+))\rangle - \frac{1}{2\hbar}\langle z - a(T_1^+), F(z - a(T_1^+))\rangle\right\} dx. \end{aligned} \tag{6.27}$$

Making the substitutions $\tilde{z} = (\tilde{x}, \tilde{y}) = z - a(T_1^+)$ the above integral can be written as

$$\begin{aligned} &\int_{\mathbb{R}} \exp\left\{\frac{i}{\hbar}\langle \xi^{\pm}, \tilde{z}\rangle - \frac{1}{2\hbar}\langle \tilde{z}, F\tilde{z}\rangle\right\} d\tilde{x} \\ = &\int_{\mathbb{R}} \exp\left\{\frac{i}{\hbar}\left[\xi_x^{\pm}\tilde{x} + \xi_y^{\pm}\tilde{y}\right] - \frac{1}{2\hbar}\left[F_{xx}\tilde{x}^2 + (F_{xy} + F_{yx})\tilde{x}\tilde{y} + F_{yy}\tilde{y}^2\right]\right\} d\tilde{x} \\ = &\exp\left\{\frac{i}{\hbar}\xi_y^{\pm}\tilde{y} - \frac{F_{yy}}{2\hbar}\tilde{y}^2 + \frac{[2i\xi_x^{\pm} - (F_{xy} + F_{yx})\tilde{y}]^2}{8F_{xx}\hbar}\right\} \\ &\qquad \times \int_{\mathbb{R}} \exp\left\{-\frac{F_{xx}}{2\hbar}\left[\tilde{x} - \frac{1}{2F_{xx}}\left(2i\xi_x^{\pm} - (F_{xy} + F_{yx})\tilde{y}\right)\right]^2\right\} d\tilde{x}. \end{aligned} \tag{6.28}$$

It is known from conditions (2.27)-(2.28) that the real part of F is a positive definite matrix and so thus we are able to evaluate this integral to get

$$(6.28) = \sqrt{\frac{2\pi\hbar}{F_{xx}}}\exp\left\{\frac{i}{\hbar}\xi_y^{\pm}\tilde{y} - \frac{F_{yy}}{2\hbar}\tilde{y}^2 + \frac{[2i\xi_x^{\pm} - (F_{xy}+F_{yx})\tilde{y}]^2}{8F_{xx}\hbar}\right\} \tag{6.29}$$

$$= \sqrt{\frac{2\pi\hbar}{F_{xx}}}\exp\left\{-\frac{(\xi_x^{\pm})^2}{2F_{xx}\hbar}\right\}\exp\left\{\left[-\frac{F_{yy}}{2\hbar} + \frac{(F_{xy}+F_{yx})^2}{8F_{xx}\hbar}\right]\tilde{y}^2\right\}$$

$$\times\exp\left\{\left[\frac{i}{\hbar}\xi_y^{\pm} - \frac{i}{2\hbar}\xi_x^{\pm}(F_{xy}+F_{yx})\right]\tilde{y}\right\}.$$

Recall that conditions (2.27)-(2.28) imply that F is symmetric and so $F_{xy} = F_{yx}$, and so from here we can see that

$$-F_{yy} + \frac{(F_{xy}+F_{yx})^2}{4F_{xx}} = -\frac{1}{F_{xx}}(\det F) \tag{6.30}$$

From here we get that

$$\langle\theta_j(\hbar,x),\phi_0(T_1^+,\hbar,x,y)\rangle_{dx} \tag{6.31}$$

$$= \frac{1}{(E_j(\hbar) - V_1(a_x(T_1^+)))^{1/4}}\sqrt{\frac{2}{(\det A(T_1^+))F_{xx}}}\exp\left\{-\frac{(\xi_x^{\pm})^2}{2F_{xx}\hbar}\right\}$$

$$\times\exp\left\{\left[-\frac{\det F}{F_{xx}}\right]\frac{\tilde{y}^2}{2\hbar}\right\}\exp\left\{\left[\frac{i}{\hbar}\xi_y^{\pm} - \frac{i}{\hbar}\xi_x^{\pm}(F_{xy})\right]\tilde{y}\right\}.$$

At this point we have to separate the the argument of the exponential into appropriate real and imaginary parts. To do this note that

$$\frac{1}{\hbar}\left\{-\frac{(\xi_x^{\pm})^2}{2F_{xx}} - \left[\frac{\det F}{F_{xx}}\right]\frac{\tilde{y}^2}{2} + i\left[\xi_y^{\pm} - \xi_x^{\pm}(F_{xy})\right]\tilde{y}\right\}$$

$$= \frac{1}{\hbar}\left\{-\frac{(\xi_x^{\pm})^2}{2F_{xx}} - \mathrm{Re}\left[\frac{\det F}{F_{xx}}\right]\frac{\tilde{y}^2}{2} - i\mathrm{Im}\left[\frac{\det F}{F_{xx}}\right]\frac{\tilde{y}^2}{2} + i\left[\xi_y^{\pm} - \xi_x^{\pm}(\mathrm{Re}F_{xy})\right]\tilde{y} + \xi_x^{\pm}(\mathrm{Im}F_{xy})\tilde{y}\right\}$$

$$= \frac{1}{\hbar}\left\{-\frac{(\xi_x^{\pm})^2}{2F_{xx}} - \mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\left[\tilde{y}^2 - \left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^{\pm}(\mathrm{Im}F_{xy})\tilde{y}\right]\right.$$

$$\left. -i\mathrm{Im}\left[\frac{\det F}{F_{xx}}\right]\frac{\tilde{y}^2}{2} + i\left[\xi_y^{\pm} - \xi_x^{\pm}(\mathrm{Re}F_{xy})\right]\tilde{y}\right\}$$

$$
\begin{aligned}
= \quad & \frac{1}{\hbar}\Bigg\{-\frac{(\xi_x^\pm)^2}{2F_{xx}} - \mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\left[\tilde{y} - \frac{1}{2}\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\right]^2 \\
& + \frac{1}{4}\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\left(\xi_x^\pm(\mathrm{Im}F_{xy})\right)^2 - i\mathrm{Im}\left[\frac{\det F}{F_{xx}}\right]\frac{\tilde{y}^2}{2} + i\left[\xi_y^\pm - \xi_x^\pm(\mathrm{Re}F_{xy})\right]\tilde{y}\Bigg\}
\end{aligned}
$$

$$
\begin{aligned}
= \quad & \frac{1}{\hbar}\Bigg\{-\frac{(\xi_x^\pm)^2}{2F_{xx}} - \mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\left[\tilde{y} - \frac{1}{2}\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\right]^2 \\
& + \frac{1}{4}\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\left(\xi_x^\pm(\mathrm{Im}F_{xy})\right)^2 - i\mathrm{Im}\left[\frac{\det F}{2F_{xx}}\right]\left[\tilde{y} - \frac{1}{2}\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\right]^2 \\
& + i\left[\xi_y^\pm - \xi_x^\pm(\mathrm{Re}F_{xy})\right]\tilde{y} - i\mathrm{Im}\left[\frac{\det F}{2F_{xx}}\right]\left[\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\tilde{y}\right] \\
& \qquad + i\mathrm{Im}\left[\frac{\det F}{2F_{xx}}\right]\left[\frac{1}{2}\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\right]^2\Bigg\}
\end{aligned}
$$

$$
\begin{aligned}
= \quad & \frac{1}{\hbar}\Bigg\{-\frac{(\xi_x^\pm)^2}{2F_{xx}} - \left[\frac{\det F}{2F_{xx}}\right]\left[\tilde{y} - \frac{1}{2}\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\right]^2 \\
& + i\left[\xi_y^\pm - \xi_x^\pm(\mathrm{Re}F_{xy})\right]\tilde{y} - i\mathrm{Im}\left[\frac{\det F}{2F_{xx}}\right]\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\tilde{y} \\
& + \frac{i}{4}\mathrm{Im}\left[\frac{\det F}{2F_{xx}}\right]\left[\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\right]^2 + \frac{1}{4}\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\left(\xi_x^\pm(\mathrm{Im}F_{xy})\right)^2\Bigg\}
\end{aligned}
$$

$$
\begin{aligned}
= \quad & \frac{1}{\hbar}\Bigg\{-\frac{(\xi_x^\pm)^2}{2F_{xx}} - \left[\frac{\det F}{2F_{xx}}\right]\left[\tilde{y} - \frac{1}{2}\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\right]^2 \\
& + i\left(\left[\xi_y^\pm - \xi_x^\pm(\mathrm{Re}F_{xy})\right] + \mathrm{Im}\left[\frac{\det F}{2F_{xx}}\right]\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\right)\left(\tilde{y} - \frac{1}{2}\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\right) \\
& + \frac{i}{2}\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\left[\left[\xi_y^\pm - \xi_x^\pm(\mathrm{Re}F_{xy})\right] + \mathrm{Im}\left[\frac{\det F}{2F_{xx}}\right]\left(\left[\mathrm{Re}\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\right] \\
& + \frac{i}{4}\mathrm{Im}\left[\frac{\det F}{2F_{xx}}\right]\left[\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\xi_x^\pm(\mathrm{Im}F_{xy})\right]^2 + \frac{1}{4}\left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}}\right]\right)^{-1}\left(\xi_x^\pm(\mathrm{Im}F_{xy})\right)^2\Bigg\}.
\end{aligned}
$$

So we have

$$
\begin{aligned}
(6.28) \quad = \quad & \frac{1}{(E_j(\hbar) - V_1(a_x(T_1^+)))^{1/4}} \sqrt{\frac{2}{(\det A(T_1^+))F_{xx}}} \\
& \times \exp\left\{ -\frac{(\xi_x^\pm)^2}{2\hbar} \left(\frac{1}{F_{xx}} - \frac{1}{2} \left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}} \right] \right)^{-1} (\mathrm{Im}(F_{xy}))^2 \right) \right\} \\
& \times \exp\left\{ \left[-\frac{\det F}{2F_{xx}\hbar} \right] \left[\tilde{y} - \frac{1}{2} \left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}} \right] \right)^{-1} \xi_x^\pm F_{xx} (\mathrm{Im}(F_{xy})) \right]^2 \right\} \\
& \times \exp\left\{ \frac{i}{\hbar} \left[\xi_y^\pm - \xi_x^\pm (\mathrm{Re} F_{xy}) + \mathrm{Im}\left[\frac{\det F}{2F_{xx}} \right] \left(\mathrm{Re}\left[\frac{\det F}{2F_{xx}} \right] \right)^{-1} \xi_x^\pm (\mathrm{Im} F_{xy}) \right] \right. \\
& \qquad \left. \times \left(\tilde{y} - \frac{1}{2} \left[\mathrm{Re}\left\{ \frac{\det F}{2F_{xx}} \right\} \right]^{-1} \xi_x^\pm (\mathrm{Im} F_{xy}) \right) \right\} \\
& \times \exp\left\{ \frac{i}{2\hbar} \left[\xi_y^\pm - \xi_x^\pm (\mathrm{Re} F_{xy}) + \frac{3}{4} \mathrm{Im}\left[\frac{\det F}{4F_{xx}} \right] \left[\mathrm{Re}\left\{ \frac{\det F}{2F_{xx}} \right\} \right]^{-1} \xi_x^\pm (\mathrm{Im} F_{xy}) \right] \right. \\
& \qquad \left. \times \left[\mathrm{Re}\left\{ \frac{\det F}{2F_{xx}} \right\} \right]^{-1} \xi_x^\pm (\mathrm{Im} F_{xy}) \right\}.
\end{aligned}
$$

This completes the proof. □

Now we show that for those energies $E_\alpha(\hbar)$ well above the ground state, the projection at a cluster time onto an eigenstate $\lambda_j(\hbar, x)$ can be given semiclassically by projecting onto $\theta_j(\hbar, x)$.

Theorem 6.32. *Assume there exists $C > 0$ such that $j \geq C\hbar^{-1}$. Let $\theta_j^\pm(\hbar, x)$ be defined as in the beginning of this section and let $\psi_{j0}(x, y, \hbar, T_1^+)$ be a modified wave-packet as defined in section (6.2) with T_1^+ chosen to be a cluster time. There exists constants $D_{j\pm}$ and $\epsilon > 0$ such that if we define $\theta_j(\hbar, x) = D_{j+}\theta_j^+(\hbar, x) + D_{j-}\theta_j^-(\hbar, x)$ there exists $0 < \nu < 1$ and $f(y)$ such that*

$$
\begin{aligned}
& \left\langle \lambda_j(\hbar, x), \phi_0(T_1^+, \hbar, x, y) \right\rangle_{dx} \\
= \quad & \left\langle \theta_j(\hbar, x), \phi_0(T_1^+, \hbar, x, y) \right\rangle_{dx} + f(y),
\end{aligned}
$$

where $\|f(y)\|_2 \leq O(\hbar^{1-\nu})$.

Proof. Let $0 < \nu < 1$, define $\chi_1(\hbar, a(T_1^+), x)$ to be the characteristic function of

$$\{x : |x - a_x(T_1^+)| < |T_1^+| \hbar^{1/2 - \nu/2}\}.$$

Define $\chi_2(\hbar, a(T_1^+), x) = 1 - \chi_1(\hbar, a(T_1^+), x)$. Now we have that

$$\int_{\mathbb{R}} \bar{\lambda}_j(\hbar, x)\phi_0(T_1^+, \hbar, x, y)dx \tag{6.33}$$

$$= \int_{\mathbb{R}} \chi_1(\hbar, a(T_1^+), x)\bar{\lambda}_j(\hbar, x)\phi_0(T_1^+, \hbar, x, y)dx \tag{6.34}$$

$$+ \int_{\mathbb{R}} \chi_2(\hbar, a(T_1^+), x)\bar{\lambda}_j(\hbar, x)\phi_0(T_1^+, \hbar, x, y)dx. \tag{6.35}$$

In accordance with Lemma (2.25) we choose $\delta = \frac{\sqrt{-2ME_j(\hbar)}}{2\hbar}$. Evaluating the term (6.34) above

$$\begin{aligned}
&\left|\int_{\mathbb{R}} \chi_2(\hbar, a(T_1^+), x)\bar{\lambda}_j(\hbar, x)\phi_0(T_1^+, \hbar, x, y)dx\right| \\
\leq\ & \|\lambda_j(\hbar, x)\|_2 \left\|\chi_2(\hbar, a(T_1^+), x)\phi_0(T_1^+, \hbar, x, y)\right\|_2 \\
\leq\ & \|\lambda_j(\hbar, x)\|_2 \left\|\chi_2(\hbar, a_x(T_1^+, x)) \exp\left\{-\frac{(x - a_x(T_1^+))}{4|A(T_1^+)|^2\hbar}\right\}\right\|_\infty \\
&\times\left\|\chi_2(\hbar, a_x(T_1^+), x)(\pi\hbar)^{-1/2}(\det A(T_1^+))^{-1/2}\right. \\
&\qquad\left.\times \exp\left\{-\frac{\langle z - a(T_1^+), B(T_1^+)A^{-1}(T_1^+)(z - a(T_1^+))\rangle}{4\hbar}\right\}\right\|_{(L^2(\mathbb{R}),dx)} \\
\leq\ & O(e^{C\hbar^{-\nu}})\left\|\chi_2(\hbar, a_x(T_1^+), x)(\pi\hbar)^{-1/2}(\det A(T_1^+))^{-1/2}\right. \\
&\qquad\left.\times \exp\left\{-\frac{\langle z - a(T_1^+), B(T_1^+)A^{-1}(T_1^+)(z - a(T_1^+))\rangle}{4\hbar}\right\}\right\|_{(L^2(\mathbb{R}),dx)}.
\end{aligned}$$

It is a quickly seen by Fubini's Theorem that

$$\left\|\left\|\chi_2(\hbar, a_x(T_1^+), x)(\pi\hbar)^{-1/2}(\det A(T_1^+))^{-1/2} \times \exp\left\{-\frac{\langle z - a(T_1^+), B(T_1^+)A^{-1}(T_1^+)(z - a(T_1^+))\rangle}{4\hbar}\right\}\right\|_{(L^2(\mathbb{R}),dx)}\right\|_{(L^2(\mathbb{R}),dy)} \leq C.$$

Let D_{j+}, D_{j-} be constants chosen in accordance with the WKB theory of section (2.2), since our energy for the bound motion is assumed to be above the bottom of the well, the set

$\{x : |x - a_x(T_1^+)| < |T_1^+|\hbar^{1/2-\nu/2}\}$ is contained in the classically acceptable region for $\hbar$ sufficiently small, and in this region

$$\lambda_j(\hbar; x) = \{D_{j+}\lambda_j^+(\hbar; x) + D_{j-}\lambda_j^-(\hbar; x)\}(1 + O(\hbar)).$$

Define

$$\lambda_j^{WKB}(\hbar; x) = D_{j+}\lambda_j^+(\hbar; x) + D_{j-}\lambda_j^-(\hbar; x).$$

Consider

$$\begin{aligned}
&\int_{\mathbb{R}} \chi_1(\hbar, a(T_1^+), x)\bar{\lambda}_j(\hbar, x)\phi_0(T_1^+, \hbar, x, y)dx \\
= &\int_{\mathbb{R}} \chi_1(\hbar, a(T_1^+), x)\bar{\lambda}_j^{WKB}(\hbar, x)(1 + O(\hbar))\phi_0(T_1^+, \hbar, x, y)dx. \\
= &\int_{\mathbb{R}} \chi_1(\hbar, a(T_1^+), x)\bar{\lambda}_j^{WKB}(\hbar, x)\phi_0(T_1^+, \hbar, x, y)dx \\
&+O(\hbar)\int_{\mathbb{R}} \chi_1(\hbar, a(T_1^+), x)\bar{\lambda}_j^{WKB}(\hbar, x)\phi_0(T_1^+, \hbar, x, y)dx.
\end{aligned}$$

It is quickly seen by Hölder's inequality and the fact that the WKB approximation is normalized that

$$\begin{aligned}
&\int_{\mathbb{R}} \chi_1(\hbar, a(T_1^+), x)\bar{\lambda}_j^{WKB}(\hbar, x)\phi_0(T_1^+, \hbar, x, y)dx \\
\leq &\left\|\phi_0(T_1^+, \hbar, x, y)\right\|_{(L^2(\mathbb{R}),dx)}.
\end{aligned} \tag{6.36}$$

Let $\mathcal{C} = \{c = \alpha a_x(T_1^+) + (1 - \alpha)x | \alpha \in [0, 1]\}$. Taking Taylor expansions with a second order remainder there exists $c_1, c_2 \in \mathcal{C}$ such that

$$\begin{aligned}
\frac{1}{(E_j(\hbar) - V_1(x))^{1/4}} &= \frac{1}{(E_j(\hbar) - V_1(a_x(T_1^+)))^{1/4}} \\
&+\left\{\frac{4V_1''(c_1)(E_j(\hbar) - V_1(c_1))^{1/4} - 5V_1'(c_1)^2}{16(E_j(\hbar) - V_1(c_1))^{3/2}}\right\}\frac{(x - a_x(T_1^+))^2}{2}
\end{aligned}$$

$$\begin{aligned}
\int_{a_x(T_1^+)}^{x} \sqrt{E_j(\hbar) - V_1(y)}dy &= \sqrt{E_j(\hbar) - V_1(a_x(T_1^+))}(x - a_x(T_1^+)) \\
&- \left\{\frac{V_1'(c_2)}{\sqrt{E_j(\hbar) - V_1(c_2)}}\right\}\frac{(x - a_x(T_1^+))^2}{2}.
\end{aligned}$$

Since $V_1'(x)$ is Lipschitz and our energy is assumed to be above the bottom of the well then for $|x - a_x(T_1^+)| < |T_1^+|\hbar^{1/2-\nu/2}$

$$\begin{aligned}\frac{1}{(E_j(\hbar) - V_1(x))^{1/4}} &= \frac{1}{(E_j(\hbar) - V_1(a_x(T_1^+)))^{1/4}} + O(\hbar^{1-\nu}) \\ \int_{a_x(T_1^+)}^{x} \sqrt{E_j(\hbar) - V_1(y)}dy &= \sqrt{E_j(\hbar) - V_1(a_x(T_1^+))}(x - a_x(T_1^+)) + O(\hbar^{3/2-3\nu/2}).\end{aligned}$$

Therefore one can see that for x in the support of $\chi_1(\hbar, x, a(T_1^+))$

$$\lambda_j^{WKB}(\hbar, x) = \theta_j(\hbar, x) + O(\hbar^{1-\nu}).$$

This implies that

$$\begin{aligned}&\left\langle \chi_1(\hbar, a_x(T_1^+), x)\lambda_j^{WKB}(\hbar, x), \phi_0(T_1^+, \hbar, x, y)\right\rangle_{dx} \\ = \; &\left\langle \chi_1(\hbar, a_x(T_1^+), x)\theta_j(\hbar, x), \phi_0(T_1^+, \hbar, x, y)\right\rangle_{dx} + O(\hbar^{1-\nu}) \left\|\phi_0(T_1^+, \hbar, x, y)\right\|_{(L^2(\mathbb{R}),dx)}.\end{aligned}$$

From here it is clear that

$$\begin{aligned}&\left\langle \lambda_j(\hbar, x), \phi_0(T_1^+, \hbar, x, y)\right\rangle_{dx} \\ = \; &\left\langle \chi_1(\hbar, a_x(T_1^+), x)\theta_j(\hbar, x), \phi_0(T_1^+, \hbar, x, y)\right\rangle_{dx} + O(\hbar^{1-\nu}) \left\|\phi_0(T_1^+, \hbar, x, y)\right\|_{(L^2(\mathbb{R}),dx)}.\end{aligned}$$

It is quickly seen that

$$\begin{aligned}&\left|\left\langle \chi_2(\hbar, a_x(T_1^+), x)\theta_j(\hbar, x), \phi_0(T_1^+, \hbar, x, y)\right\rangle_{dx}\right| \\ \leq \; &\|\theta_j(\hbar, x))\|_2 \|\chi_2(\hbar, a_x(T_1^+, x))\phi_0(T_1^+, \hbar, x, y)\|_{(L^2(\mathbb{R}),dx)}.\end{aligned}$$

This can be taken care of in the same way as (6.36), proving the theorem. □

This result also holds for low quantum numbers with a couple of adjustments in the proof. We also note that due to equation (2.50) we do not lose any more accuracy in $\hbar$ than we already have by using the quasistates rather than the actual eigenstates.

At this point the classical mechanics for the free particle for positive infinite times will be given for $t > T_1^+$ by

$$\mathcal{A}_{yy}(t) = \mathcal{A}_{yy}(T_1^+) + ti\mathcal{B}_{yy}(T_1^+)/\mu \tag{6.37}$$

$$\mathcal{B}_{yy}(t) = \mathcal{B}_{yy}(T_1^+) \tag{6.38}$$

$$a_y^{out_j}(t) = a_y^{out_j}(T_1^+) + t\eta_y^{out_j}(T_1^+)/\mu \tag{6.39}$$

$$\eta_y^{out_j}(t) = \eta_y^{out_j}(T_1^+) \tag{6.40}$$

$$S_y(t) = \frac{(t - T_1^+)\left(\eta_y^{out_j}\right)^2}{2\mu} + \frac{\eta_y^2(T_1^+)}{2\mu} \tag{6.41}$$

with the conditions at T_1^+ given by

$$\mathcal{A}_{yy}(T_1^+) = \mathcal{C}\frac{(\det A(T_1^+))\left[B(T_1^+)A^{-1}(T_1^+)\right]_{xx}}{2} \tag{6.42}$$

$$\mathcal{B}_{yy}(T_1^+) = \mathcal{C}\frac{(\det A(T_1^+))\det\left[B(T_1^+)A^{-1}(T_1^+)\right]}{2} \tag{6.43}$$

$$a_y^{out_j}(T_1^+) = a_y(T_1^+) + \frac{1}{2}\left[\mathrm{Re}\left\{\frac{\det B(T_1^+)A^{-1}(T_1^+)}{2\left(B(T_1^+)A^{-1}(T_1^+)\right)_{xx}}\right\}\right]^{-1} \tag{6.44}$$

$$\times\left(\mp\sqrt{(2M)(E_j(\hbar)-V_1(a_x(t)))}+\eta_x(t))(\mathrm{Im}(B(t)A^{-1}(t)_{xy})\right)$$

$$\eta_y^{out_j}(T_1^+) = \left\{\eta_y(T_1^+) - \left(\mp\sqrt{(2M)(E_j(\hbar)-V_1(a_x(T_1^+)))}+\eta_x(T_1^+)\right)\right. \tag{6.45}$$

$$\times\left[\mathrm{Re}[B(T_1^+)A^{-1}(T_1^+)]_{xy} + \mathrm{Im}\frac{\det B(T_1^+)A^{-1}(T_1^+)}{2B(T_1^+)A^{-1}(T_1^+)_{xx}}\left(\mathrm{Re}\frac{\det B(T_1^+)A^{-1}(T_1^+)}{2B(T_1^+)A^{-1}(T_1^+)_{xx}}\right)^{-1}\right.$$

$$\left.\left.\times\mathrm{Im}[B(T_1^+)A^{-1}(T_1^+)]_{xy}\right]\right\}. \tag{6.46}$$

$\mathcal{C}$ is chosen so that

$$\mathcal{A}\bar{\mathcal{B}} + \bar{\mathcal{A}}\mathcal{B} = 2. \tag{6.47}$$

From Lemmas (6.27) and (6.33) The wavepacket is approximated by

$$\Phi_0^{j\pm}(\mathcal{A}_{yy}(t),\mathcal{B}_{yy}(t),\hbar,a_y^{out_j}(t),\eta_y^{out_j}(t),y) \tag{6.48}$$

$$= \frac{(\pi\hbar)^{1/4}\mathcal{C}^{1/2}}{(E_j(\hbar)-V_1(a_x(T_1^+)))^{1/4}} \times \phi_0(\mathcal{A}_{yy}(t),\mathcal{B}_{yy}(t),\hbar,a_y^{out_j}(t)\eta_y^{out_j}(t),y)$$

$$\times\exp\left\{-\frac{(\mp\sqrt{(2M)(E_j(\hbar)-V_1(a_x(T_1^+)))}+\eta_x(T_1^+))^2}{2\hbar}\right.$$

$$\left.\times\left(\frac{1}{[B(T_1^+)A^{-1}(T_1^+)]_{xx}} - \frac{1}{2}\left[\mathrm{Re}\frac{\det B(T_1^+)A^{-1}(T_1^+)}{2(B(T_1^+)A^{-1}(T_1^+))_{xx}}\right]^{-1}(\mathrm{Im}(B(T_1^+)A^{-1}(T_1^+))_{xy}))^2\right)\right\}$$

$$\times\exp\left\{\frac{-i}{2\hbar}\left[\tilde{\eta}_y^{out_j}(T_1^+) + \frac{3}{4}\mathrm{Im}\frac{\det B(T_1^+)A^{-1}(T_1^+)}{B(T_1^+)A^{-1}(T_1^+)_{xx}}\left[\mathrm{Re}\frac{\det B(T_1^+)A^{-1}(T_1^+)}{2B(T_1^+)A^{-1}(T_1^+)_{xx}}\right]^{-1}\mathrm{Im}[B(T_1^+)A^{-1}(T_1^+)]_{xy}\right]\right.$$

$$\left.\times\left[\mathrm{Re}\left\{\frac{\det B(T_1^+)A^{-1}(T_1^+)}{2B(T_1^+)A^{-1}(T_1^+)_{xx}}\right\}\right]^{-1}\left(\mp\sqrt{(2M)(E_j(\hbar)-V_1(a_x(T_1^+)))}+\eta_x(T_1^+)\right)(\mathrm{Im}B(T_1^+)A^{-1}(T_1^+)_{xy})\right\}.$$

Now we define the constants $C_j^{1\pm}(\hbar)$ to be given by

$$\begin{aligned}
C_j^{1\pm}(\hbar) &= \langle \Phi_0^{j\pm}(t,\hbar,y), \Phi_0^{j\pm}(t,\hbar,y)\rangle_{dy} \qquad (6.49)\\
&= \frac{(\pi\hbar)^{1/2}|\mathcal{C}|}{(E_j(\hbar) - V_1(a_x(T_1^+)))^{1/2}}\\
&\quad \exp\Bigg\{-\Bigg\{\frac{(\mp\sqrt{(2M)(E_j(\hbar) - V_1(a_x(T_1^+)))} + \eta_x(T_1^+))^2}{\hbar}
\end{aligned}$$

$$\times \mathrm{Re}\Bigg(\frac{1}{[B(T_1^+)A^{-1}(T_1^+)]_{xx}} - \frac{1}{2}\left(\mathrm{Re}\frac{\det B(T_1^+)A^{-1}(T_1^+)}{2(B(T_1^+)A^{-1}(T_1^+))_{xx}}\right)^{-1}(\mathrm{Im}(B(T_1^+)A^{-1}(T_1^+))_{xy}))^2\Bigg)\Bigg\}\Bigg\}.$$

At this point we need to show that

$$\mathrm{Re}\Bigg(\frac{1}{[B(T_1^+)A^{-1}(T_1^+)]_{xx}} - \frac{1}{2}\left(\mathrm{Re}\frac{\det B(T_1^+)A^{-1}(T_1^+)}{2(B(T_1^+)A^{-1}(T_1^+))_{xx}}\right)^{-1}(\mathrm{Im}(B(T_1^+)A^{-1}(T_1^+))_{xy}))^2\Bigg) > 0.$$

We simplify as before letting $F = BA^{-1}$. The above quantity is equivalent to

$$\begin{aligned}
&\frac{\mathrm{Re}F_{xx}}{|F_{xx}|^2} - \frac{|F_{xx}|^2(\mathrm{Im}F_{xy})^2}{[\mathrm{Re}\det F][\mathrm{Re}F_{xx}] + [\mathrm{Im}(\det F)][\mathrm{Im}F_{xx}]}\\
&= \frac{\mathrm{Re}F_{xx}\{[\mathrm{Re}\det F][\mathrm{Re}F_{xx}] + [\mathrm{Im}(\det F)][\mathrm{Im}F_{xx}]\} - |F_{xx}|^4(\mathrm{Im}F_{xy})^2}{|F_{xx}|^2[\mathrm{Re}\det F][\mathrm{Re}F_{xx}] + |F_{xx}|^2[\mathrm{Im}(\det F)][\mathrm{Im}F_{xx}]}\\
&= \frac{\mathrm{Re}F_{xx}\{[\mathrm{Re}\det F][\mathrm{Re}F_{xx}] + [\mathrm{Im}(\det F)][\mathrm{Im}F_{xx}]\}}{|F_{xx}|^2[\mathrm{Re}\det F][\mathrm{Re}F_{xx}] + |F_{xx}|^2[\mathrm{Im}(\det F)][\mathrm{Im}F_{xx}]}\\
&\quad - \frac{|F_{xx}|^4(\mathrm{Im}F_{xy})^2}{|F_{xx}|^2[\mathrm{Re}\det F][\mathrm{Re}F_{xx}] + |F_{xx}|^2[\mathrm{Im}(\det F)][\mathrm{Im}F_{xx}]}
\end{aligned}$$

The first term above is known to be positive definite since it symplifies to be

$$\frac{\mathrm{Re}F_{xx}}{|F_{xx}|^2}.$$

We will now show that the first term is dominant for large time. Considering just the numerators in the above expression we have

$$= \{[\mathrm{Re}\det F][\mathrm{Re}F_{xx}]^2 + [\mathrm{Re}F_{xx}][\mathrm{Im}(\det F)][\mathrm{Im}F_{xx}]\} - |F_{xx}|^4(\mathrm{Im}F_{xy})^2. \qquad (6.50)$$

For large times $B(t) = B_+$ and $A(t) = A_+ + iB_+t$ therefore we have

$$\begin{aligned}
\mathrm{Re}\det F &= \frac{(\mathrm{Re}\det B)(\mathrm{Re}\det A) + (\mathrm{Im}\det B)(\mathrm{Im}\det A)}{|\det A|^2}\\
&= \frac{C}{t^2} + O(t^{-2}).
\end{aligned}$$

We quickly see that $(\mathrm{Re}F_{xx})^2$ is asymptotic to t^{-1} since there exists $a, b, c, d, e, f \in \mathbb{R}$ such that

$$\begin{aligned}\mathrm{Re}F_{xx} &= \mathrm{Re}\frac{a+ib}{c+dt+ie+ift} \\ &= \frac{ac+adt+be+bft}{(c+dt)^2+(e+ft)^2}\end{aligned}$$

Following this reasoning it is easy to see that for large t the first two terms together in (6.51) are asymptotic to t^{-3} and the second term in (6.51) is asymptotic to t^{-6} and thus (6.51) > 0 for large t. Now Φ_0^j defined by equation (6.17) is given by

$$\Phi_0^j \;=\; D_k^{j+}\Phi_0^{j+} + D_k^{j-}\Phi_0^{j-} + O(\hbar^{1-\nu}) \tag{6.51}$$

where the $D_k^{j\pm}$ are given by section (2.2) and $\nu > 0$ is arbitrary. Now for large enough positive times the approximation will be given by

$$\left\{\sum_j \exp\left\{\tfrac{i}{\hbar}(S_y(t) - tE_j(\hbar))\right\}\lambda_j(\hbar, x_k)\Phi_0^j(\mathcal{A}_{yy}(t), \mathcal{B}_{yy}(t), \hbar, a_y^{out_j}(t), \eta_y^{out_j}, y)\right\}. \tag{6.52}$$

Interpretation of 6.49: Equation (6.49) is quite interesting as it approximates with at most an error of $O(\hbar^{2-2\nu})$ the probability of being in any particular state. Initially our intuition was that in the semiclassical limit the final state would be given to first order by the exact classical orbit. While it is still centered around the classical path, due to the inherent uncertainty of the semiclassical mechanics we get a spread over those paths that are near the classical orbit and the probability of being in the state corresponding to the actual classical orbit is less than we first expected. We get a significant contribution from those states such that

$$\left(\mp\sqrt{(2M)(E_j(\hbar) - V_1(a_x(T_1^+)))} + \eta_x(T_1^+)\right)^2 = O(\hbar). \tag{6.53}$$

All states that satisfy (6.54) occur with probability on the order of $\hbar^{1/2}$.

The Bohr Sommerfeld analysis of section (2.4) implies that given two quasiclassical energies $E_k(\hbar)$ and $E_j(\hbar)$, we have

$$|E_k(\hbar) - E_j(\hbar)| \leq C|k-j|\hbar \tag{6.54}$$

where C is a constant. Suppose E_c is the classical energy in the bound state direction. Consider a transverse energy $E(\hbar)$ such that $|E(\hbar) - E_c| = O(\hbar^{1/2})$. By taking a second order Taylor series about E_c we have

$$\begin{aligned}
&\left(\eta_x(T_1^+) \pm \sqrt{(2M)(E(\hbar) - V_1(a_x(T_1^+)))}\right)^2 \qquad (6.55)\\
= &\left(\eta_x(T_1^+) \pm \sqrt{(2M)(E_c - V_1(a_x(T_1^+)))}\right)^2 + O(|E(\hbar) - E_c|^2)\\
= &\ O(|E(\hbar) - E_c|^2).
\end{aligned}$$

In the above we have taken the appropriate sign to correspond to the classical momentum the other term will be constant in the semiclassical limit making the corresponding terms in (6.52) negligible. We can now see that there are $O(\hbar^{-1/2})$ quasiclassical states $E(\hbar)$ within $C\hbar^{1/2}$ of E_c that will contribute on the order of $\hbar^{1/2}$. Therefore our wavefunction will be on the order of 1. In addition any WKB state that corresponds to an energy E_j such that $|E_j - E_c| > C\hbar^{1/2}$ will have negligible contribution to the sum (6.52) in the limit $\hbar \to 0$.

Theorem 6.56. *Let $[a, b] \subset (V_1(a_{x_1}(T_1^-)), 0)$, suppose that η_{y_-}, the momentum of the incoming free particle, is given such that the total energy, as defined in section 6.4, $E \in [a, b]$. Let $h_1 = h_1(\hbar)$ be the Hamiltonian for the sub-system* (23) *that is in a bound state as $t \to \infty$. Let $E_j(\hbar) \in \sigma_{pp}(h_1)$ be the set of Eigenvalues for h_1 with corresponding Eigenvectors $\lambda_j(\hbar, x)$. Let Φ_0 be determined by equation (6.17). Then*

$$\begin{aligned}
&\Bigg\| e^{iS(T_1^+)/\hbar}\phi_0(A(T_1^+), B(T_1^+), \hbar, a(T_1^+), \eta(T_1^+), x, y) \qquad (6.57)\\
&- \sum_{\{E_j \in \sigma_p(h_1)\}} e^{i(S_y^\alpha(T_1^+) - T_1^+ E_j)/\hbar}\tilde{\lambda}_j(\hbar, x)\Phi_0^j(\mathcal{A}_{yy}(T_1^+), \mathcal{B}_{yy}(T_1^+), \hbar, a_y^{out_j}(T_1^+), \eta_y^{out_j}(T_1^+), y)\Bigg\|_{L^2(\mathbb{R}^2)}\\
\leq &\ O(\hbar^\delta)
\end{aligned}$$

for some $\nu > 0$ and $\tilde{\lambda}_j(\hbar, x) = e^{-iT_1^+[E_c - E_j(\hbar)]/\hbar}\lambda_j(\hbar, x)$.

Proof. By standard spectral theory and conservation of energy arguments it is clear that we can pick a cluster time T_1^+ large enough so that

$$\begin{aligned}
&e^{iS(T_1^+)/\hbar}\phi_0(A(T_1^+), B(T_1^+), \hbar, a(T_1^+), \eta(T_1^+), x, y) =\\
&\sum_{E_j \in \sigma_p(h_1) \cap [a,b]} \Bigg\{ e^{iS_y(T_1^+)/\hbar}\lambda_j(\hbar, x)\\
&\qquad \times \langle \lambda_j(\hbar, x), \phi_0(A(T_1^+), B(T_1^+), \hbar, a(T_1^+), \eta(T_1^+), x, y)\rangle_{dx} \Bigg\} + O(\hbar)\\
= &\sum_{E_j \in \sigma_p(h_1) \cap [a,b]} \Bigg\{ e^{i[S_y - T_1^+ E_j(\hbar)]/\hbar}\tilde{\lambda}_j(\hbar, x)\langle \lambda_j(\hbar, x), \phi_0(A(t), B(t), \hbar, a(t), \eta(t), x, y)\rangle_{dx} \Bigg\} + O(\hbar).
\end{aligned}$$

We note that by chosing t to be a cluster time T_1^+ we have

$$\begin{aligned} S(T_1^+) &= \frac{\eta_y^2 T_1^+}{2\mu} + \int_0^{T_1^+} \frac{\eta_x^2(t)}{2M} - V_1(a_x(t))dt \\ &= S_y(T_1^+) - E_c T_1^+. \end{aligned}$$

E_c is the energy of the orbit given by classical mechanics and η_y is the momentum in the y direction that is given by classical mechanics. Let $\delta > 0$ and define

$$\begin{aligned} A &= \left\{\sigma_p(h_1) \cap \left[E_c - \hbar^{1/2-\delta/2}, E_c + \hbar^{1/2-\delta/2}\right]\right\} \\ B &= \sigma_p(h_1)\backslash A. \end{aligned} \tag{6.58}$$

Let μ_{h_1} be the expected value of $h_1(\hbar)$ as measured in the state $\phi_0(A(T_1^+), B(T_1^+), \hbar, a(T_1^+), \eta(T_1^+), x, y)$. In the appendix to chapter 2 we showed that the expected value of the energy operator will be $O(\hbar)$ within the classical energy and so if $|E_j(\hbar) - E_c| = O(\hbar)$ then $|E_j(\hbar) - \mu_{h_1}| = O(\hbar)$. Suppressing the T_1^+ dependence and noting that by theorem (6.32) we can say

$$\sum_{E_j \in A} e^{i[S - T_1^+ E_j(\hbar)]/\hbar} \tilde{\lambda}_j(\hbar, x) \langle \lambda_j(\hbar, x), \phi_0(A, B, \hbar, a, \eta, x, y)\rangle_{dx} \tag{6.59}$$

$$= \sum_{E_j \in A} \left\{ e^{i[S - T_1^+ E_j(\hbar)]/\hbar} \tilde{\lambda}_j(\hbar, x) \langle \theta_j(\hbar, x), \phi_0(A, B, \hbar, a, \eta, x, y)\rangle_{dx} + \hbar^{1-\nu} f_j(y) \right\} \tag{6.60}$$

where there exists constants c_j such that $\|f_j(y)\|_2 \leq c_j$. By the argument given to interpret (6.48) only $C\hbar^{-1/2}$ of the inner product terms contribute on the order of $\hbar^{1/2}$. Therefore the total error in (6.61) is bounded by $C_4 \hbar^{1/2-\nu} f(y)$ where $\|f(y)\|_2 \leq F$, for F constant. Now consider

$$\sum_{E_j \in B} e^{i[S - T_1^+ E_j(\hbar)]/\hbar} \tilde{\lambda}_j(\hbar, x) \langle \lambda_j(\hbar, x), \phi_0(A, B, \hbar, a, \eta, x, y)\rangle_{dx}. \tag{6.61}$$

At this point we appeal to the Chebyshev inequality [21], of probability theory which states that the probability that an observed value y of an observable quantity Y differs from the mean μ_y by ϵ is given by

$$P[|y - \mu_y| > \epsilon] \leq \frac{\sigma_y^2}{\epsilon^2}.$$

The variance of $h_1 \otimes I$ in the state $\phi_0(x, y, T_1^+)$ is given by

$$\sigma^2 g(y) = \langle \phi_0(x, y, T_1^+), \{(h_1 - \mu_{h_1})^2 \otimes I\} \phi(x, y, T_1^+)\rangle_{dx}$$

We showed in the appendix to chapter 2 that the variance of a wavepacket is $O(\hbar)$. So it follows that the probability that $h_1 \otimes I$ yields an object $E_j(\hbar) g_j(y) \in L^2(\mathbb{R})$ where $|E_j(\hbar) - \mu_{h_1}| > \hbar^{1/2-\delta/2}$ for any given $\delta > 0$. It follows that the total probability that we have a state in B is $O(\hbar^\delta)$. $\square$

6.8 Existence and Uniqueness of Semiclassical Scattering States

In this section we show how a semiclassical wave-operator can be constructed for a dynamical system that exhibits separation as $t \to \pm\infty$. Let $H(\hbar)$, and $H_1(\hbar)$ be defined as before with Unitary propogator $U^\hbar(t) = e^{-itH(\hbar)/\hbar}$.

Theorem 6.62. *Let $V_i(\cdot)$ be compactly supported for $i = 1, 2, 3$. Let T_1^- be a cluster time. Then for $t < T_1^-$, there exists C, C_1, ϵ all positive such that*

$$\begin{aligned} &\|U^\hbar(t - T_1^-)\psi_{j0}(x, y, \hbar, T_1^-) - \psi_{j0}(x, y, \hbar, t)\|_{L^2(\mathbb{R}^2)} \\ \leq\ & C \exp\left\{-\frac{C_1|T_1^-|}{\hbar}\right\} + C|T_1^-|^{-1/2}\hbar^{-5/4}\exp\left\{-C_1\hbar^{-2\epsilon}\right\}. \end{aligned} \tag{6.63}$$

This theorem is existence and uniqueness of scattering states for the modified semiclassics. We prove this for negative times in the (x_1, y_1) coordinates but we can just as easily prove this for large positive time or in the (x_3, y_3) coordinates. We note that asymptotic completeness will be an inherited quality of asymptotic completeness for the classical system. The basic premise here follows the same premise as that of Theorem (4.1) in that we remove the portion of the wave-packet that has zero asymptotic momentum. This portion is of order $\hbar^{1/2}$.

Proof. Define

$$\begin{aligned} \tilde{\phi}_0(t, \hbar, y) &= \left\{1 + \frac{(y - a_y(t))iB_{yy}}{A_{yy}(t)\eta_y}\right\}\phi_0(t, \hbar, y) \\ &= \phi_0(t, \hbar, y) + i\sqrt{\frac{\hbar}{2}}\frac{B_{yy}}{\eta_y}\phi_1(t, \hbar, y). \end{aligned}$$

where for ease in notation we have suppressed the dependence on the classical mechanics. Now define

$$\tilde{\psi}_{j0}(x, y, \hbar, t) = \exp\left\{\frac{i}{\hbar}(S_y(t) - tE_j(\hbar))\right\}\lambda_j(\hbar, x)\tilde{\phi}_0(t, \hbar, y).$$

So we have

$$\begin{aligned} &\|U^\hbar(t - T_1^-)\psi_{j0}(x, y, \hbar, T_1^-) - \psi_{j0}(x, y, \hbar, t)\|_{L^2(\mathbb{R}^2)} \leq \\ &\left\|U^\hbar(t - T_1^-)\tilde{\psi}_{j0}(x, y, \hbar, T_1^-) - \exp\left\{\frac{i}{\hbar}(S_y(t) - tE_j(\hbar))\right\}\lambda_j(\hbar, x)\tilde{\phi}_0(t, \hbar, y)\right\|_2 \\ +\ & k\sqrt{\frac{\hbar}{2}}\left\|U^\hbar(t - T_1^-)\psi_{j1}(x, y, \hbar, T_1^-) - \exp\left\{\frac{i}{\hbar}(S_y(t) - tE_j(\hbar))\right\}\lambda_j(\hbar, x)\phi_1(t, \hbar, y)\right\|_2 \end{aligned}$$

Due to the unitarity of $U^\hbar(\cdot)$ and since the wavepacket and the eigenstate both are normalized the second norm above is seen to be bounded by 2. Now we see that

$$
\begin{aligned}
&\left\| U^\hbar(t-T_1^-)\tilde{\psi}_{j0}(x,y,\hbar,T_1^-) - \exp\left\{\frac{i}{\hbar}(S_y(t)-tE_j(\hbar))\right\}\lambda_j(\hbar,x)\phi_0(t,\hbar,y)\right\|_2 \\
= &\left\| U^\hbar(-T_1^-)\tilde{\psi}_{j0}(x,y,\hbar,T_1^-) - \exp\left\{\frac{i}{\hbar}(tH(\hbar)+S_y(t)-tE_j(\hbar))\right\}\lambda_j(\hbar,x)\tilde{\phi}_0(t,\hbar,y)\right\|_2 \\
= &\left\| \int_{T_1^-}^t \frac{\partial}{\partial s}\left\{\tilde{\psi}_{j0}(x,y,\hbar,T_1^-) - \exp\left\{\frac{i}{\hbar}(sH(\hbar)+S_y(s)-sE_j(\hbar))\right\}\lambda_j(\hbar,x)\tilde{\phi}_0(s,\hbar,y)\right\} ds\right\|_2 \\
= &\left\| \int_{T_1^-}^t -i\hbar^{-1}\left\{H(\hbar)-E_j(\hbar)\right\}\exp\left\{\frac{i}{\hbar}(sH(\hbar)+S_y(s)-sE_j(\hbar))\right\}\lambda_j(\hbar,x)\tilde{\phi}_0(s,\hbar,y)\right. \\
&\left. - \exp\left\{\frac{i}{\hbar}(sH(\hbar)-sE_j(\hbar)\right\}\lambda_j(\hbar,x)\left\{\frac{\partial}{\partial s}\left[\exp\left\{\frac{i}{\hbar}S_y(s)\right\}\tilde{\phi}_0(s,\hbar,y)\right]\right\} ds\right\|_2 \\
= &\left\| \int_{T_1^-}^t -i\hbar^{-1}\left\{H(\hbar)-E_j(\hbar)\right\}\exp\left\{\frac{i}{\hbar}(sH(\hbar)+S_y(s)-sE_j(\hbar))\right\}\lambda_j(\hbar,x)\tilde{\phi}_0(s,\hbar,y)\right. \\
&\left. +i\hbar^{-1}\exp\left\{\frac{i}{\hbar}(sH(\hbar)-sE_j(\hbar)\right\}\lambda_j(\hbar,x)\left[H_1(\hbar)-h_1(\hbar)\right]\exp\left\{\frac{i}{\hbar}S_y(s)\right\}\tilde{\phi}_0(s,\hbar,y)ds\right\|_2 \\
\leq\ &\hbar^{-1}\int_{T_1^-}^t \left\|\exp\left\{\frac{i}{\hbar}(sH)(\hbar)-sE_j(\hbar))\right\}\left[h_1(\hbar)-E_j(\hbar)\right]\lambda_j(\hbar,x)\exp\left\{\frac{i}{\hbar}S_y(s)\right\}\tilde{\phi}_0(s,\hbar,y)\right\|_2 ds \\
&+\hbar^{-1}\int_{T_1^-}^t \left\|\exp\left\{\frac{i}{\hbar}(sH(\hbar)-sE_j(\hbar))\right\}\left[V_2(y+x/2)+V_3(y-x/2)-W_2(y,a(s))-W_3(y,a(s))\right]\right. \\
&\left. \times\lambda_j(\hbar,x)\exp\left\{\frac{i}{\hbar}S_y(s)\right\}\tilde{\phi}_0(s,\hbar,y)\right\|_2 ds \\
\leq\ &\hbar^{-1}\int_{T_1^-}^t \left\|\left[V_2(y+x/2)-W_2(y,a(s))\right]\lambda_j(\hbar,x)\tilde{\phi}_0(s,\hbar,y)\right\|_2 \\
&+\left\|\left[V_3(y-x/2)-W_3(y,a(s))\right]\lambda_j(\hbar,x)\tilde{\phi}_0(s,\hbar,y)\right\|_2 ds.
\end{aligned}
$$

Let $\mu<1$, $\epsilon\in(0,1/6)$ and define $\chi_{11}(\hbar,a(t),x,y)$ to be the characteristic function of

$$\{(x,y): |y-a_y(t)|\leq\mu(1+|a_y(t)|-x/2)\hbar^{1/2-\epsilon}, |x|\leq|a_y(t)|\}.$$

Define $\chi_{12}(\hbar,a(t),x,y)$ to be the characteristic function of

$$\{(x,y): |y-a_y(t)|\geq\mu(1+|a_y(t)|-x/2)\hbar^{1/2-\epsilon}, |x|\leq|a_y(t)|\}.$$

Define $\chi_2(\hbar, a(t), x, y)$ to be the characteristic function of

$$\{|x| \geq |a_y(t)|\}.$$

Then

$$\begin{aligned}
& \hbar^{-1} \int_{T_1^-}^{t} \left\| \left[V_2(y + x/2) - W_2(y, a(s)) \right] \lambda_j(\hbar, x) \tilde{\phi}_0(s, \hbar, y) \right\|_2 ds \\
\leq \; & \hbar^{-1} \int_{T_1^-}^{t} \left\| \chi_{11}(\hbar, a(s), x, y) \left[V_2(y + x/2) - W_2(y, a(s)) \right] \lambda_j(\hbar, x) \tilde{\phi}_0(s, \hbar, y) \right\|_2 ds \\
& + \hbar^{-1} \int_{T_1^-}^{t} \left\| \chi_{12}(\hbar, a(s), x, y) \left[V_2(y + x/2) - W_2(y, a(s)) \right] \lambda_j(\hbar, x) \tilde{\phi}_0(s, \hbar, y) \right\|_2 ds \\
& + \hbar^{-1} \int_{T_1^-}^{t} \left\| \chi_2(\hbar, a(s), x, y) \left[V_2(y + x/2) - W_2(y, a(s)) \right] \lambda_j(\hbar, x) \tilde{\phi}_0(s, \hbar, y) \right\|_2 ds \\
= \; & \{ I(s) + II(s) + III(s) \}
\end{aligned}$$

Lemma (6.67) shows that $I(s) = 0$, Lemma (6.68) shows that $II(s) \leq C|T_1^-|^{-1/2}\hbar^{-5/4}e^{-C_1\hbar^{-2\epsilon}}$, and Lemma (6.73) shows that $III(s) \leq C\hbar^{-1} \exp\left\{ \frac{-C_1|T_1^-|}{\hbar^{1/2}} \right\}$, where C, C_1 are constants. $\square$

Next we give the technicalities used in the proof of theorem (6.86). We start by presenting a simple Lemma used a few times in the calculations.

Lemma 6.64. *Let $f(\cdot), g(\cdot) \in L^2(\mathbb{R})$ and $c \in \mathbb{R}, c \neq 0$ then*

$$\|f(y + cx)g(y)\|_{L^2(\mathbb{R}^2)} \leq |c|^{-1/2} \|f\|_{L^2(\mathbb{R})} \|g\|_{L^2(\mathbb{R})}$$

Proof. Without loss of generality assume $c > 0$

$$\begin{aligned}
\|f(y + cx)g(y)\|_{L^2(\mathbb{R}^2)} &= \left\{ \int_{\mathbb{R}} \left(\int_{\mathbb{R}} |f(y + cx)g(y)|^2 dy \right) dx \right\}^{1/2} \\
&\leq \left\{ \int_{\mathbb{R}} |g(y)|^2 \left(\int_{\mathbb{R}} |f(y + cx)|^2 dx \right) dy \right\}^{1/2} \\
&= \left\{ \int_{\mathbb{R}} |g(y)|^2 dy \left(\int_{\mathbb{R}} |f(u)|^2 \frac{du}{c} \right) \right\}^{1/2} \\
&\leq c^{-1/2} \|f\|_{L^2(\mathbb{R})} \|g\|_{L^2(\mathbb{R})}.
\end{aligned}$$

$\square$

Lemma 6.65. *For the cluster time* T_1^- *and* $s < T_1^-$ *we have*

$$\left\| \chi_{11}(\hbar, a(s), x, y) \left[V_2(y + x/2) - W_2(y, a(s)) \right] \lambda_j(\hbar, x) \tilde{\phi}_0(s, \hbar, y) \right\|_2 = 0$$

where $\chi_{11}(\hbar, a(s), x, y)$ *and* ϵ *are defined in the proof of theorem (6.86).*

Proof. Define

$$\begin{aligned} U_{a(t),2}(x, y) &= V_2(a_y(t) + x/2) + V_2'(a_y(t) + x/2)(y - a_y(t)) \\ &\quad + \frac{1}{2} V_2''(a_y(t) + x/2)(y - a_y(t))^2 \\ U_{a(t),3}(x, y) &= V_3(a_y(t) - x/2) + V_3'(a_y(t) - x/2)(y - a_y(t)) \\ &\quad + \frac{1}{2} V_3''(a_y(t) - x/2)(y - a_y(t))^2. \end{aligned}$$

Now we have

$$\begin{aligned} & \|\chi_{11}(\hbar, a(s), x, y)\{V_2(y + x/2) - W_2(y, a(s))\}\lambda_j(\hbar, x)\tilde{\phi}_0(A_{yy}(s), B_{yy}(s), a_y(s), \eta_y(s), y)\|_2 \\ \leq \;& \|\chi_{11}(\hbar, a(s), x, y)\{V_2(y + x/2) - U_{a(s),2}(x, y)\}\lambda_j(\hbar, x)\tilde{\phi}_0(A_{yy}(s), B_{yy}(s), a_y(s), \eta_y(s), y)\|_2 \\ + \;& \|\chi_{11}(\hbar, a(s), x, y)\{U_{a(s),2}(x, y) - W_2(y, a(s))\}\lambda_j(\hbar, x)\tilde{\phi}_0(A_{yy}(t), B_{yy}(t), a_y(t), \eta_y(t), y)\|_2 \end{aligned}$$

First we analyze

$$\|\chi_{11}(\hbar, a(s), x, y)\{V_2(y + x/2) - U_{a(s),2}(x, y)\}\lambda_j(\hbar, x)\tilde{\phi}_0(A_{yy}(s), B_{yy}(s), a_y(s), \eta_y(s), y)\|_2.$$

Let

$$|a_y(s) - y| \leq \mu(1 + |a_y(s)| - |x|/2)\hbar^{1/2-\epsilon}$$

and $|x| \leq |a_y(s)|$. By Taylor's theorem there exists $y_B \in \{r a_y(s) + (1 - r)y : r \in [0, 1]\}$ such that

$$V_2(y + x/2) - U_{a(s),2}(y, x) = \frac{V_2(y_B + x/2)(y - a_y(s))^3}{3}$$

and

$$|y_B + x/2| + |a_y(s) - y_B| \geq |a_y(s) + x/2|.$$

Furthermore

$$|a_y(s)| - |x|/2 \geq 0.$$

All of this implies that

$$\begin{aligned} (|y_B + x/2|) &\geq |a_y(s)| - |a_y(s) - y_B| - |x|/2 \\ &\geq |a_y(s)| - |x|/2 - \mu(1 + |a_y(s)| - |x|/2) \\ &\geq (1 - \mu)(1 + |a_y(s)| - |x|/2) - 1 \\ &\geq (1 - \mu)(1 + |a_y(s)|/2) - 1 \end{aligned}$$

Therefore $\chi_{11}(\hbar, a(s), x, y)\{V_2(y+x/2) - U_{a(s),2}(y,x)\} = 0$ for $s < T_1^-$ and so

$$\|\chi_{11}(\hbar, a(s), x, y)\{V_2(y+x/2) - U_{a(s),2}(x,y)\}\lambda_j(\hbar, x)\tilde{\phi}_0(A_{yy}(s), B_{yy}(s), a_y(s), \eta_y(s), y)\|_2 = 0$$

for $s < T_1^-$. Now look at the portion

$$\|\chi_{11}(\hbar, a(s), x, y)\{U_{a(s),2}(x,y) - W_2(y, a(s))\}\lambda_j(\hbar, x)\tilde{\phi}_0(A_{yy}(s), B_{yy}(s), a_y(s), \eta_y(s), y)\|_2$$

Since our potentials are compactly supported, and since both $|x|$ and $|a_x(s)|$ are less than $|a_y(s)|$ in our region, this norm is zero for $s < T_1^-$. □

The following Lemma follows the analysis of Lemma 4.11

Lemma 6.66. *Let $\chi_{12}(\hbar, a(s), x, y)$ and ϵ be as defined in Theorem (6.64). Let T_1^- be the negative cluster time. Then there exists $C, C_1, \nu > 0$, such that for $s < T_1^-$*

$$\left\|\chi_{12}(\hbar, a(s), x, y)\left[V_2(y+x/2) - W_2(y, a(s))\right]\lambda_j(\hbar, x)\tilde{\phi}_0(s, \hbar, y)\right\|_2 \leq C\hbar^{-1/4}e^{-C_1\hbar^{-2\epsilon}}|s|^{-3/2}.$$

Proof. Since $|x| \leq |a_y(t)|$ and $|y - a_y(t)| \geq \mu(1+|a_y(t)|-|x|/2)\hbar^{1/2-\epsilon}$ we have that $|y-a_y(t)| \geq \mu(1+|a_y(t)|/2)\hbar^{1/2-\epsilon}$. Now we have following the argument in Theorem (4.1)

$$\begin{aligned} & \|\chi_{12}(\hbar, a(s), x, y)V_2(y+x/2)\tilde{\psi}_{i0}(x, y, \hbar, s)\|_{L^2(\mathbb{R}^2)} \\ \leq\ & \exp\{-C'\hbar^{-2\epsilon}\} \\ & \times\left\|\chi_{12}(\hbar, a(s), x, y)\lambda_j(\hbar, x)V_2(y+x/2)\left\{1 + \frac{(y-a_y(s))iB_{yy}}{A_{yy}(s)\eta_y}\right\}\right. \\ & \left.\qquad\qquad \times(\pi\hbar)^{-1/4}(A_{yy}(s))^{-1/2}\exp\left\{\frac{-(y-a_y(s))^2}{4|A_{yy}(s)|^2\hbar}\right\}\right\|_{L^2(\mathbb{R}^2)} \end{aligned}$$

Now we can see in a manner similar to that of lemma (4.11) that

$$\begin{aligned} & \left\|\chi_{12}(\hbar, a(s), x, y)\lambda_j(\hbar, x)V_2(y+x/2)\left\{1 + \frac{(y-a_y(s))iB_{yy}}{A_{yy}(s)\eta_y}\right\}\right. \\ & \left.\qquad\qquad \times(\pi\hbar)^{-1/4}(A_{yy}(s))^{-1/2}\exp\left\{\frac{-(y-a_y(s))^2}{4|A_{yy}(s)|^2\hbar}\right\}\right\|_{L^2(\mathbb{R}^2)} \\ \leq\ & |A_{yy}(s)\eta_y|^{-1}\left\|\chi_{12}(\hbar, a(s), x, y)\lambda_j(\hbar, x)V_2(y+x/2)\left\{A_{yy}(s)\eta_y + (y-a_y(s))iB_{yy}\right\}\right. \\ & \left.\qquad\qquad \times(\pi\hbar)^{-1/4}(A_{yy}(s))^{-1/2}\exp\left\{\frac{-(y-a_y(s))^2}{4|A_{yy}(s)|^2\hbar}\right\}\right\|_{L^2(\mathbb{R}^2)} \end{aligned}$$

Since beyond the cluster times the classical mechanics is propogated freely, given $s < T_1^-$

$$\begin{aligned}
& \Bigg\| \chi_{12}(\hbar, a(s), x, y)\lambda_j(\hbar, x)V_2(y + x/2)\Big\{ A_{yy}(s)\eta_y + (y - a_y(s))iB_{yy} \Big\} \\
& \qquad \times (\pi\hbar)^{-1/4}(A_{yy}(s))^{-1/2} \exp\left\{ \frac{-(y - a_y(s))^2}{4|A_{yy}(s)|^2\hbar} \right\} \Bigg\|_{L^2(\mathbb{R}^2)} \\
= & \Bigg\| \chi_{12}(\hbar, a(s), x, y)\lambda_j(\hbar, x)V_2(y + x/2) \left\{ (A_{yy} + iB_{yy}s)\eta_y + (y - a_y - \eta_y s)iB_{yy} \right\} \\
& \qquad \times (\pi\hbar)^{-1/4}(A_{yy}(s))^{-1/2} \exp\left\{ \frac{-(y - a_y(s))^2}{4|A_{yy}(s)|} \right\} \Bigg\|_{L^2(\mathbb{R}^2)}
\end{aligned}$$

It is a quick matter to see that

$$\begin{aligned}
& \Bigg\| \chi_{12}(\hbar, a(s), x, y)\lambda_j(\hbar, x)V_2(y + x/2)A_{yy}\eta_y \\
& \qquad \times (\pi\hbar)^{-1/4}(A_{yy}(s))^{-1/2} \exp\left\{ \frac{-(y - a_y(s))^2}{4|A_{yy}(s)|^2\hbar} \right\} \Bigg\|_{L^2(\mathbb{R}^2)} \\
\leq\ & C\hbar^{-1/4}|A_{yy}(s)|^{-1/2}\|\lambda_j(\hbar, x)V_2(y + x/2)\|_{L^2(\mathbb{R}^2)} \\
\leq\ & C'\hbar^{-1/4}|A_{yy}(s)|^{-1/2}\|\lambda_j(\hbar, x)\|_{L^2(\mathbb{R})}\|V_2(u)\|_{L^2(\mathbb{R})} \\
\leq\ & C''\hbar^{-1/4}|A_{yy}(s)|^{-1/2}.
\end{aligned}$$

Where we have used Lemma (6.64) above. Now we consider

$$\begin{aligned}
& \Bigg\| \chi_{12}(\hbar, a(s), x, y)\lambda_j(\hbar, x)V_2(y + x/2)iB_{yy}(y - a_y) && (6.67) \\
& \qquad \times (\pi\hbar)^{-1/4}(A_{yy}(s))^{-1/2} \exp\left\{ \frac{-(y - a_y(s))^2}{4|A_{yy}(s)|^2\hbar} \right\} \Bigg\|_{L^2(\mathbb{R}^2)} \\
\leq\ & C\hbar^{-1/4}|A_{yy}(s)|^{-1/2} \Big\| \chi_{12}(\hbar, a(s), x, y)\lambda_j(\hbar, x)V_2(y + x/2)iB_{yy}(y - a_y) \Big\|_{L^2(\mathbb{R}^2)} && (6.68) \\
\leq\ & C'\hbar^{-1/4}|A_{yy}(s)|^{-1/2}\|\lambda_j(\hbar, x)\|_{L^2(\mathbb{R})}\|V_2(u)(u - a_y)\|_{L^2(\mathbb{R})} && (6.69) \\
& + C''\hbar^{-1/4}|A_{yy}(s)|^{-1/2}\|(x/2)\lambda_j(\hbar, x)\|_{L^2(\mathbb{R})}\|V_2(u)\|_{L^2(\mathbb{R})}. && (6.70)
\end{aligned}$$

At this point the lemma is proven since $A_{yy}(s) = A_{yy} + iB_{yy}s$ and noting that $x\lambda_j(\hbar, x)$ and $(u - a_y)V_2(u)$ are in L^2. The potentials the compactly supported and so by our choice of T_1^- we have that $W_2(y, a(s))$ is zero. □

Lemma 6.71. *There exist positive constants C_1, C_2, such that for $\hbar$ sufficiently small and all $t < T_1^-$, the negative cluster time, we have*

$$\hbar^{-1} \int_{T_1^-}^{t} \Big\| \chi_2(\hbar, a(s), x, y) \left[V_2(y + x/2) - W_2(y, a(s)) \right] \lambda_j(\hbar, x)\tilde{\phi}_0(s, \hbar, y) \Big\|_2 ds \leq C_1\hbar^{-1} \exp\left\{ \frac{-C_2|T_1^-|}{\hbar^{1/2}} \right\}.$$

In the above, $\chi_2(\hbar, a(s), x, y)$ *is defined as in theorem (6.64).*

Proof. Recall that for $t < T_1^-$ then $|x| > |a_y(t)| > \frac{|\eta_y t|}{2}$. Furthermore in accordance with Lemma (2.25) we choose $\delta = \frac{\sqrt{-2MV_1(a_x(T_1^-))}}{2\hbar}$.

$$\begin{aligned}
& \hbar^{-1} \int_{T_1^-}^{t} \left\| \chi_2(\hbar, a(s), x, y) \left[V_2(y + x/2) - W_2(y, a(s)) \right] \lambda_j(\hbar, x) \tilde{\phi}_0(s, \hbar, y) \right\|_2 ds \quad (6.72) \\
\leq & \ \hbar^{-1} \int_{T_1^-}^{t} C e^{-\delta|\eta_y s|/2} \left\| \chi_2(\hbar, a(s), x, y) e^{\delta|x|} \lambda_j(\hbar, x) \tilde{\phi}_0(s, \hbar, y) \right\|_2 ds \\
\leq & \ \hbar^{-1} \int_{T_1^-}^{t} C \exp\left\{ \frac{-\delta|\eta_y s|}{2} \right\} \left\| \chi_2(\hbar, a(s), x, y) e^{\delta|x|} \lambda_j(\hbar, x) \tilde{\phi}_0(s, \hbar, y) \right\|_2 ds \\
\leq & \ \hbar^{-1} \int_{T_1^-}^{t} C \exp\left\{ \frac{C_2 s}{\hbar^{1/2}} \right\} ds \\
\leq & \ C_1 \left\{ \exp\left\{ \frac{C_2 s}{\hbar^{1/2}} \right\} \right\}_t^{T_1^-} \\
= & \ C_1 \left\{ \exp\left\{ \frac{C_2 T_1^-}{\hbar^{1/2}} \right\} - \exp\left\{ \frac{C_2 t}{\hbar^{1/2}} \right\} \right\} \\
\leq & \ C_1 \exp\left\{ \frac{-C_2 |T_1^-|}{\hbar^{1/2}} \right\} \quad (6.73)
\end{aligned}$$

where C_1 and C_2 are positive constants. □

Chapter 7

Possibilities for Future research

There are quite a few directions in which the research presented here can be extended. One possible direction is the use of wave-packets to give a semiclassical approximation for Schrödinger equations with Hamiltonians that are more general than the ones given in section (2.4). In [12] it is shown that one can use the wave-packet construction to give exact solutions for time dependent Hamiltonians that are quadratic in position and momentum. Using this technique we should be able to provide a semiclassical description for the problem of a particle in a magnetic field. Another possibility worth investigating is the that of writing the wave-packets in polar or spherical coordinates for two and three dimensional problems.

The results of chapter four can also be extended. It should be straightforward to describe scattering of the higher-order, $j > 0$ wave-packets in one and two dimensions. Investigation in this direction has begun. In [6] scattering of these wave packets is discussed for the Coulomb potential. These results are limited to $n = 3$. One could investigate scattering of more general long range potentials.

There are many possible ways to extend the results of chapter 6. Our results are limited to pairwise potentials that are compactly supported. We plan to investigate further the results of classical scattering theory for the N-body problem in hopes of proving that the approximation is valid for more general problems. Extension possibilities include extending to pairwise potentials that are short-range. We also hope to study the problem with more bodies. It may be possible to show that the collinear problem is a good approximation to certain 3 dimensional problems.

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