Exponentially Accurate Semiclassical Dynamics: Propagation, Localization, Ehrenfest Times, Scattering, and More General States

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November 26, 1999

Abstract

We prove six theorems concerning exponentially accurate semiclassical quantum mechanics. Two of these theorems are known results, but have new proofs. Under appropriate hypotheses, they conclude that the exact and approximate dynamics of an initially localized wave packet agree up to exponentially small errors in $\hbar$ for finite times and for Ehrenfest times. Two other theorems state that for such times the wave packets are localized near a classical orbit up to exponentially small errors. The fifth theorem deals with infinite times and states an exponentially accurate scattering result. The sixth theorem provides extensions of the other five by allowing more general initial conditions.

MSC: 81Q20
Keywords: Semiclassical methods, quantum dynamics, exponential asymptotics

*Partially Supported by National Science Foundation Grant DMS–9703751.

1 Introduction

This paper is devoted to proving several theorems concerning exponentially accurate approximations to solutions of the time-dependent Schrödinger equation

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

in the semiclassical limit $\hbar \to 0$.

The semiclassical approximation of quantum dynamics has been the object of several recent investigations from different points of view. One approach uses coherent state initial conditions and approximates the evolved wave packet by suitable linear combinations of coherent states. Another approach considers the Heisenberg evolution of suitable bounded observables and approximates the corresponding operators by means of Egoroff's theorem. The goal of both approaches is to produce accurate, computable approximations as $\hbar$ goes to zero, for as long a time interval as possible. In scattering situations the time interval is the whole real line.

There are several results concerning the propagation of certain coherent states for finite time intervals. Early results [14, 7] constructed approximate solutions that were accurate up to $O(\hbar^{1/2})$ errors. Later approximations were constructed with $O(\hbar^{l/2})$ errors for any l [8, 9, 5, 16]. Very recently, approximations were constructed with errors of exponential order $O(\mathrm{e}^{-\Gamma/\hbar})$ with $\Gamma > 0$ in [11] (see also [22]).

The validity of the corresponding approximations for time intervals of length $O(\ln(1/\hbar))$, the so-called Ehrenfest time-scale, has been established up to $O(\hbar^{l/2})$ errors in [5], and up to $O(e^{1/\hbar^{\alpha}})$ errors with $0 < \alpha < 1$ in [11] . There is physical intuition and evidence that the Ehrenfest time scale is the natural limit for the validity of coherent state type approximations. This issue is studied in detail for the quantized Baker and Cat maps in [2].

Approximations have been constructed for infinite times in the context of scattering theory for coherent states. Approximate solutions with errors of order $O(\hbar^{1/2})$, uniformly in time, are produced in [7]. This yields approximations for the scattering matrix with errors that are also $O(\hbar^{1/2})$. Related results for another class of states can be found in [20, 21].

Corresponding results for the approximation of observables in the Heisenberg picture can be found in [18] for approximations with $O(\hbar^{l/2})$ errors for any l for finite times. Approximations with exponentially small errors both for finite times and for Ehrenfest times are constructed in [1] and [3].

The exponentially accurate results mentioned above, and those we present below, are obtained for Hamiltonians that satisfy certain analyticity conditions. The approximations are generated by optimal truncation of asymptotic series.

For further information, we refer the reader to the review articles [4, 19, 15, 12].

The present paper is concerned with the propagation of coherent states in the spirit of the first approach described above. We present a new construction of approximate solutions to the time dependent Schrödinger equation that is an alternative to the one presented in [11].

The new expansion has several advantages. In addition to being exponentially accurate up to the Ehrenfest time scale (Theorems 3.1 and 3.3), it allows us to extend our previous

results in four separate directions:
1. We get exponentially precise localization properties for both the approximation and the exact solution for both finite times and Ehrenfest times (Theorems 3.2 and 3.4).
2. We get exponentially accurate information on the semiclassical limit of the scattering matrix for suitable short range potentials (Theorem 3.5).
3. The new algorithm is superior for numerical computation. The work done to construct the approximate wave function for one value of $\hbar$ is used for the construction for all smaller values of $\hbar$. This should be contrasted with the construction of [11] where every calculation must be redone for each value of $\hbar$.
4. The results in [11] concern the propagation of initial coherent states given by a linear combination of a finite number N of elementary coherent states. We can control the new approximation as a function of N, which also allows us to extend the validity of all previous results to a more general set of initial states (Theorem 3.6). In this case however, the algorithm requires the computation of different quantities as $\hbar$ varies.

The technical difference between the present construction and the one in [11] is the following: In both papers, we use a suitable time dependent basis to convert the PDE (1.1) into an infinite system of ODE's for the expansion coefficients in that basis of the solution to the Schrödinger equation. In [11] we then construct the approximate solution by approximating this infinite system by a finite system, which we solve exactly. In the new approach, we substitute an *a priori* expansion in powers of $\hbar^{1/2}$ into the original infinite system of ODE's. We construct our approximate solution by keeping a finite number of terms. This turns out to be quite efficient.

The new approximation also plays a vital role in the construction of an exponentially accurate time–dependent Born–Oppenheimer approximation [13].

2 Coherent States and Classical Dynamics

We begin this section by recalling the definition of the coherent states $\phi_j(A,\, B,\, \hbar,\, a,\, \eta,\, x)$ described in detail in [10]. A more explicit, but more complicated definition is given in [9].

We adopt the standard multi-index notation. A multi-index $j\,=\,(j_1,\, j_2,\, \dots,\, j_d)$ is a d-tuple of non-negative integers. We define $|j| = \sum_{k=1}^d j_k,\quad x^j = x_1^{j_1} x_2^{j_2} \cdots x_d^{j_d}$,
$j! = (j_1!)(j_2!)\cdots(j_d!)$, and $D^j = \frac{\partial^{|j|}}{(\partial x_1)^{j_1}(\partial x_2)^{j_2}\cdots(\partial x_d)^{j_d}}$.

Throughout the paper we assume $a \in I\!\!R^d$, $\eta \in I\!\!R^d$ and $\hbar > 0$. We also assume that A and B are $d \times d$ complex invertible matrices that satisfy

$$\begin{aligned} A^t\, B\, -\, B^t\, A &= 0, \\ A^*\, B\, +\, B^*\, A &= 2\, I. \end{aligned} \tag{2.1}$$

These conditions guarantee that both the real and imaginary parts of BA^{-1} are symmetric. Furthermore, $\mathrm{Re}\, BA^{-1}$ is strictly positive definite, and $(\mathrm{Re}\, BA^{-1})^{-1} = A\, A^*$.

Our definition of $\varphi_j(A,\, B,\, \hbar,\, a,\, \eta,\, x)$ is based on the following raising operators that are defined for $m = 1, 2, \ldots, d$.

$$\mathcal{A}_m(A, B, \hbar, a, \eta)^* \;=\; \frac{1}{\sqrt{2\hbar}} \left[\sum_{n=1}^d \overline{B}_{n\,m}\,(x_n - a_n) \;-\; i\,\sum_{n=1}^d \overline{A}_{n\,m}\,(-i\hbar\frac{\partial}{\partial x_n} - \eta_n) \right].$$

The corresponding lowering operators $\mathcal{A}_m(A, B, \hbar, a, \eta)$ are their formal adjoints.

These operators satisfy commutation relations that lead to the properties of the $\phi_j(A,\, B,\, \hbar,\, a,\, \eta,\, x)$ that we list below. The raising operators $\mathcal{A}_m(A, B, \hbar, a, \eta)^*$ for $m = 1, 2, \ldots, d$ commute with one another, and the lowering operators $\mathcal{A}_m(A, B, \hbar, a, \eta)$ commute with one another. However,

$$\mathcal{A}_m(A, B, \hbar, a, \eta)^*\, \mathcal{A}_n(A, B, \hbar, a, \eta) \;-\; \mathcal{A}_n(A, B, \hbar, a, \eta)\, \mathcal{A}_m(A, B, \hbar, a, \eta)^* \;=\; \delta_{m,n}.$$

Definition For the multi-index $j = 0$, we define the normalized complex Gaussian wave packet (modulo the sign of a square root) by

$$\phi_0(A,\, B,\, \hbar,\, a,\, \eta,\, x) \;=\; \pi^{-d/4}\, \hbar^{-d/4}\, (\det(A))^{-1/2}$$
$$\times \quad \exp\left\{ -\langle\, (x-a),\, B\,A^{-1}\,(x-a)\,\rangle/(2\hbar) \;+\; i\,\langle\, \eta,\, (x-a)\,\rangle/\hbar \right\}.$$

Then, for any non-zero multi-index j, we define

$$\phi_j(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot\,) \;=\; \frac{1}{\sqrt{j!}}\; (\,\mathcal{A}_1(A, B, \hbar, a, \eta)^*)^{j_1}\;\; (\,\mathcal{A}_2(A, B, \hbar, a, \eta)^*)^{j_2}\;\cdots$$
$$\times\; (\,\mathcal{A}_d(A, B, \hbar, a, \eta)^*)^{j_d}\;\; \phi_0(A\,, B,\, \hbar,\, a,\, \eta,\, \cdot\,).$$

Properties 1. For $A = B = I$, $\hbar = 1$, and $a = \eta = 0$, the $\phi_j(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot\,)$ are just the standard Harmonic oscillator eigenstates with energies $|j| + d/2$.

2. For each admissible A, B, $\hbar$, a, and η, the set $\{\, \phi_j(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot\,)\,\}$ is an orthonormal basis for $L^2(I\!\!R^d)$.

3. The raising operators can also be given by another formula that was omitted from [10] in the multi-dimensional case. If we set

$$g(A,\, B,\, \hbar,\, a,\, x) \;=\; \exp\left\{ -\langle\, (x-a),\, \left(BA^{-1}\right)^*\,(x-a)\,\rangle/(2\hbar) \;-\; i\langle\, \eta,\, (x-a)\,\rangle/\hbar \right\},$$

then we have

$$(\,\mathcal{A}_m(A, B, \hbar, a, \eta)^*\,\psi\,)\,(x)$$
$$=\; -\,\sqrt{\frac{\hbar}{2}}\; \frac{1}{g(A,\, B,\, \hbar,\, a,\, x)}\; \sum_{n=1}^d\; \overline{A}_{n\,m}\, \frac{\partial}{\partial x_n}\; (\,g(A,\, B,\, \hbar,\, a,\, x)\,\psi(x)\,)\,.$$

4. In [9], the state $\phi_j(A,\, B,\, \hbar,\, a,\, \eta,\, x)$ is defined as a normalization factor times

$$\mathcal{H}_j(A;\, \hbar^{-1/2}\,|A|^{-1}\,(x-a))\;\, \phi_0(A,\, B,\, \hbar,\, a,\, \eta,\, x).$$

Here $\mathcal{H}_j(A;\, y)$ is a recursively defined $|j|^{\rm th}$ order polynomial in y that depends on A only through U_A, where $A = |A|\, U_A$ is the polar decomposition of A.

5. By scaling out the $|A|$ and $\hbar$ dependence and using Remark 3 above, one can show that $\mathcal{H}_j(A;\, y)\, \mathrm{e}^{-y^2/2}$ is an (unnormalized) eigenstate of the usual Harmonic oscillator with energy $|j| + d/2$.

6. When the dimension d is 1, the position and momentum uncertainties of the $\phi_j(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot\,)$ are $\sqrt{(j+1/2)\hbar}\;|A|$ and $\sqrt{(j+1/2)\hbar}\;|B|$, respectively. In higher dimensions, they are bounded by $\sqrt{(|j|+d/2)\hbar}\;\|A\|$ and $\sqrt{(|j|+d/2)\hbar}\;\|B\|$, respectively.

7. When we approximately solve the Schrödinger equation, the choice of the sign of the square root in the definition of $\phi_0(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot\,)$ is determined by continuity in t after an arbitrary initial choice.

8. We prove below that the matrix elements of $(x-a)^m$ satisfy

$$\begin{aligned} & |\,\langle\, \phi_j(A,\, B,\, \hbar,\, a,\, \eta,\, x),\, (x-a)^m\, \phi_k(A,\, B,\, \hbar,\, a,\, \eta,\, x) \rangle\,| \\ \leq\;\; & \hbar^{|m|/2}\, (\sqrt{2}d)^{|m|}\, \|A\|^{|m|}\, \sqrt{(|k|+1)(|k|+2)\cdots(|k|+|m|)}, \end{aligned}$$

and

$$\langle\, \phi_j(A,\, B,\, \hbar,\, a,\, \eta,\, x),\, (x-a)^m\, \phi_k(A,\, B,\, \hbar,\, a,\, \eta,\, x)\,\rangle \;=\; 0, \quad \text{if} \quad \Big|\, |j| - |k| \,\Big| > |m|. \tag{2.2}$$

We now assume that the potential $V : I\!R^d \to I\!R$ is smooth and bounded below. Our semiclassical approximations depend on solutions to the following classical equations of motion

$$\begin{aligned} \dot a(t) &= \eta(t), \\ \dot \eta(t) &= -\nabla V(a(t)), \\ \dot A(t) &= i\, B(t), \\ \dot B(t) &= i\, V^{(2)}(a(t))\, A(t), \\ \dot S(t) &= \frac{\eta(t)^2}{2} - V(a(t)), \end{aligned} \tag{2.3}$$

where $V^{(2)}$ denotes the Hessian matrix for V, and the initial conditions $A(0)$, $B(0)$, $a(0)$, $\eta(0)$, and $S(0)=0$ satisfy (2.1).

The matrices $A(t)$ and $B(t)$ are related to the linearization of the classical flow through the following identities:

$$\begin{aligned} A(t) &= \frac{\partial a(t)}{\partial a(0)}\, A(0) \,+\, i\, \frac{\partial a(t)}{\partial \eta(0)}\, B(0), \\ B(t) &= \frac{\partial \eta(t)}{\partial \eta(0)}\, B(0) \,-\, i \frac{\partial \eta(t)}{\partial a(0)}\, A(0). \end{aligned}$$

Because V is smooth and bounded below, there exist global solutions to the first two equations of the system (2.3) for any initial condition. From this, it follows immediately that the remaining three equations of the system (2.3) have global solutions. Furthermore, it is not difficult [8, 9] to prove that conditions (2.1) are preserved by the flow.

The usefulness of our wave packets stems from the following important property [10]. If we decompose the potential as

$$V(x) \;=\; W_a(x) \;+\; Z_a(x) \;\equiv W_a(x) \;+\; (V(x) - W_a(x)), \tag{2.4}$$

where $W_a(x)$ denotes the second order Taylor approximation (with the obvious abuse of notation)

$$W_a(x) \;\equiv\; V(a) \;+\; V^{(1)}(a)\,(x-a) \;+\; V^{(2)}(a)\,(x-a)^2/2.$$

then for all multi-indices j,

$$\begin{aligned} & i\,\hbar\,\frac{\partial}{\partial t}\,\left[\mathrm{e}^{iS(t)/\hbar}\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)\right] \\ & = \;\left(-\,\frac{\hbar^2}{2}\,\Delta\,+\,W_{a(t)}(x)\right)\,\left[\mathrm{e}^{iS(t)/\hbar}\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)\right], \end{aligned} \tag{2.5}$$

if $A(t)$, $B(t)$, $a(t)$, $\eta(t)$, and $S(t)$ satisfy (2.3). In other words, our semiclassical wave packets φ_j exactly take into account the kinetic energy and quadratic part $W_{a(t)}(x)$ of the potential when propagated by means of the classical flow and its linearization around the classical trajectory selected by the initial conditions.

In the rest of the paper, whenever we write $\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)$, we tacitly assume that $A(t), B(t), a(t), \eta(t)$, and $S(t)$ are solutions to (2.3) with initial conditions satisfying (2.1).

3 The Main Results

In this section, we list our results concerning the propagation of semiclassical wave packets. The first is the construction of an approximate wave function that agrees with the exact wave function up to an exponentially small error. The construction is quite explicit. It depends on the somewhat arbitrary choice of a parameter $g>0$.

The precise result is summarized in the following theorem:

Theorem 3.1 *Suppose $V(x)$ is real and bounded below for $x\in I\!R^d$. Assume V extends to an analytic function in a neighborhood of the region $S_\delta\;=\;\{\,z\;:\;|\,Im\;z_j\,|\;\leq\;\delta\,\}$ and satisfies $|V(z)|\;\leq\;M\,\exp\left(\tau|z|^2\right)$ for $z\in S_\delta$ and some positive constants M and τ.*

Fix T, choose a classical orbit $a(t)$ for $0\leq t\leq T$, and consider an arbitrary normalized coherent state of the form

$$\psi(x,0,\hbar)=\sum_{|j|\leq J}\,c_j(0)\,\phi_j(A(0),B(0),\hbar,a(0),\eta(0),x).$$

There exists a number $G>0$, such that for each choice of the parameter $g\in(0,\,G)$, there exists an exact solution to the Schrödinger equation,

$$i\,\hbar\,\frac{\partial\Psi}{\partial t}\;\;=\;\;-\,\frac{\hbar^2}{2}\,\Delta\,\Psi\;\;+\;V\,\Psi,$$

with $\Psi(x,0,\hbar)=\psi(x,0,\hbar)$*, that agrees with the approximate solution*

$$\psi(x,t,\hbar) \;=\; e^{iS(t)/\hbar} \sum_{|j|\leq J+3g/\hbar-3} c_j(t,\hbar)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x),$$

up to an error whose $L^2(I\!\!R^d)$ *norm is bounded by* $C\exp\{-\gamma_g/\hbar\}$*, with* $\gamma_g>0$*. Furthermore, the complex coefficients* $c_j(t,\hbar)$ *are determined by an explicit procedure.*

The second result shows that the approximate wave function of Theorem 3.1 is concentrated within an arbitrarily small distance of the classical path up to an exponentially small error if g is chosen sufficently small.

Theorem 3.2 *Suppose that the hypotheses of Theorem 3.1 are satisfied and that* $b>0$ *is given. For sufficiently small values of the parameter* $g>0$*, the wave packet* $\psi(x,t,\hbar)$ *is localized within a distance* b *of* $a(t)$*, up to an error* $\exp\{-\Gamma_g/\hbar\}$*, with* $\Gamma_g>0$*, in the sense that*

$$\left(\int_{|x-a(t)|>b} |\psi(x,t,\hbar)|^2\,dx\right)^{1/2} \;\leq\; \exp\{-\Gamma_g/\hbar\}.$$

Next, we turn to the validity of the approximation and its localization properties on the Ehrenfest time scale, i.e. when T is allowed to increase with $\hbar$ as $\ln(1/\hbar)$.

Theorem 3.3 *Suppose the assumptions of Theorem 3.1 are satisfied except that the upper bound on* V *is replaced by* $|V(z)|\leq M\exp(\tau|z|)$ *for* $z\in S_\delta$ *and some positive constants* M *and* τ*. Further, assume the existence of a constant* $N>0$ *and a positive Lyapunov exponent* λ *so that* $\|A(t)\|\leq N\exp(\lambda t)$*, for all* $t\geq 0$*. Then, for sufficiently small* $T'>0$*, there exist constants* $C'>0$*,*$\gamma'>0$*,* $\sigma\in(0,1)$*, and* $\sigma'\in(0,1)$*, and an exact solution to the Schrödinger equation that agrees with the approximation*

$$\psi(x,t,\hbar) \;=\; e^{iS(t)/\hbar} \sum_{|j|\leq J+3/\hbar^{\sigma'}-3} c_j(t,\hbar)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x),$$

up to an error whose norm is bounded by $C'\exp\{-\gamma'/\hbar^{\sigma}\}$*, whenever* $0\leq t\leq T'\ln(1/\hbar)$*. Moreover, if* τ *can be taken arbitrarily small, we can chose* $T'=\frac{1}{6\lambda}(1-\epsilon)$ *where* ϵ *is arbitrarily small.*

Remark: The semiclassical approximation of observables in the Heisenberg picture holds for any $T'<2/(3\lambda)$, when $\tau<<1$, as shown recently in [3]. That time interval is longer than those for which a localized coherent state can approximate the evolution of an initial coherent state, which is characterized by $T'<1/(2\lambda)$. See [2] for a study of related issues on quantized hyperbolic maps on the torus.

Theorem 3.4 *Suppose the hypotheses of Theorem 3.3 are satisfied and that* $b>0$ *is given. Then, for sufficiently small* $T'>0$*, there exist* $\Gamma'>0$*,* $\sigma\in(0,1)$*, and* $\sigma'\in(0,1)$*, such that the approximation of Theorem 3.3 satisfies*

$$\left(\int_{|x-a(t)|>b} |\psi(x,t,\hbar)|^2\,dx\right)^{1/2} \;\leq\; \exp\{-\Gamma'/\hbar^{\sigma}\},$$

whenever $0 \leq t \leq T' \ln(1/\hbar)$.
Moreover, if τ *can be taken arbitrarily small, we can chose* $T' = \frac{1}{6\lambda}(1-\epsilon)$ *where* ϵ *is arbitrarily small.*

We also explore the validity of the approximation in a scattering framework and its consequences on the corresponding semiclassical approximation of the scattering matrix $S(\hbar)$. This requires assumptions on the decay of the potential and its derivatives at infinity.

For scattering theory, we assume V satisfies the following decay hypothesis.

D: *There exist* $\beta > 1$, $v_0 > 0$, *and* $v_1 > 0$, *such that for all* $x \in I\!\!R^d$ *and all multi-indices* $m \in \mathbf{N}^d$,

$$D^m V(x) \;\leq\; \frac{v_0\, v_1^{|m|}\, m!}{\langle x\rangle^{\beta+|m|}}, \tag{3.1}$$

where $\langle x\rangle \;=\; \sqrt{1+x^2}$.

Theorem 1.2 of [7] shows that under the hypothesis D, the solution of the classical equations (2.3) satisfies the following asymptotic estimates:

For any $a_- \in I\!\!R^d$, $0 \neq \eta_- \in I\!\!R^d$ such that $(a_-,\, \eta_-) \in I\!\!R^{2d} \backslash \mathcal{E}$, where $\mathcal{E} \subseteq \{(a_-,\, \eta_-) \in I\!\!R^{2d} : \eta_- \neq 0\}$ is closed and of Lebesgue measure zero in $I\!\!R^d$, there exists $(a_+,\, \eta_+) \in I\!\!R^{2d}$, $\eta_+ \neq 0$, and $S_+ \in I\!\!R$ such that

$$\begin{aligned}
\lim_{t\to\pm\infty} |a(t) - a_\pm - \eta_\pm t| &= 0,\\
\lim_{t\to\pm\infty} |\eta(t) - \eta_\pm| &= 0,\\
\lim_{t\to-\infty} |S(t) - t\eta_-^2/2| &= 0,\\
\lim_{t\to+\infty} |S(t) - S_+ - t\eta_+^2/2| &= 0.
\end{aligned} \tag{3.2}$$

Moreover, for any $d\times d$ matrices $(A_-,\, B_-)$ satisfying condition (2.1), there exist matrices $(A_+,\, B_+) \in M_d(\mathbb{C})^2$ satisfying (2.1), such that

$$\begin{aligned}
\lim_{t\to\pm\infty} \|A(t) - A_\pm - iB_\pm t\| &= 0,\\
\lim_{t\to\pm\infty} \|B(t) - B_\pm\| &= 0.
\end{aligned} \tag{3.3}$$

Our assumption D implies that V is short range. It follows that if $H_0(\hbar) \;=\; -\,\dfrac{\hbar^2}{2}\,\Delta$, then the wave operators defined by

$$\Omega^{\mp}(\hbar) \;=\; s - \lim_{s\to\pm\infty} \mathrm{e}^{iH(\hbar)s/\hbar}\, \mathrm{e}^{-iH_0(\hbar)s/\hbar} \tag{3.4}$$

exist and have identical ranges equal to the absolutely continuous subspace of $H(\hbar)$. As a result, the scattering matrix

$$S(\hbar) \;=\; \Omega^-(\hbar)^*\, \Omega^+(\hbar) \tag{3.5}$$

is unitary.

Theorem 3.5 *Suppose $d \geq 3$ and assume hypothesis D. Let $(a_-, \eta_-) \in I\!\!R^{2d} \backslash \mathcal{E}$ and $(A_-, B_-) \in M_d(I\!\!\!C)^2$ satisfy condition (2.1). Let $c_j(-\infty) \in I\!\!\!C$, for $j \in \mathbf{N}^d$, with $|j| \leq J$, such that $\sum_{|j| \leq J} |c_j(-\infty)|^2 = 1$. Then, there exist $(a_+, \eta_+) \in I\!\!R^{2d}$, $(A_+, B_+) \in M_d(I\!\!\!C)^2$ satisfying (2.1), $S_+ \in I\!\!R$ and explicit coefficients $c_j(+\infty, \hbar) \in I\!\!\!C$, for all $j \in \mathbf{N}^d$, with $|j| \leq \tilde{J}_\hbar$ with $\tilde{J}_\hbar = J + 3g/\hbar - 3$ such that for some $\gamma > 0$, $C > 0$, $g > 0$ (depending on the the classical data), the states defined by*

$$\begin{aligned} \Phi_-(A_-, B_-, \hbar, a_-, \eta_-, x) &= \sum_{|j| \leq J} c_j(-\infty) \phi_j(A_-, B_-, \hbar, a_-, \eta_-, x) \\ \Phi_+(A_+, B_+, \hbar, a_+, \eta_+, x) &= e^{iS_+/\hbar} \sum_{|j| \leq \tilde{J}_\hbar} c_j(+\infty, \hbar) \phi_j(A_+, B_+, \hbar, a_+, \eta_+, x) \end{aligned} \tag{3.6}$$

satisfy

$$\| S(\hbar)\, \Phi_-(A_-, B_-, \hbar, a_-, \eta_-, \cdot) \;-\; \Phi_+(A_+, B_+, \hbar, a_+, \eta_+, \cdot) \|_{L^2(I\!\!R^d)} \;\leq\; C\, e^{-\gamma/\hbar},$$

if $\hbar$ is small enough.

Finally, we address the question of the generalization of the initial coherent state, whose evolution can be controlled up to exponential accuracy in the different settings considered above.

For $(a, \eta) \in I\!\!R^{2d}$, we define $\Lambda_h(a, \eta)$ to be the operator

$$(\Lambda_\hbar(a, \eta) f)(x) \;=\; \hbar^{-d/2}\, \mathrm{e}^{i\langle \eta,\, (x-a) \rangle/\hbar}\, f((x-a)/\sqrt{\hbar}).$$

We define a dense set $\mathcal{C}$ in $L^2(I\!\!R^d)$, that is contained in the set $\mathcal{S}$ of Schwartz functions, by

$$\begin{aligned} \mathcal{C} \;=\; \Bigg\{ & f(x) = \sum_j c_j\, \phi_j(I\!\!I, I\!\!I, 1, 0, 0, x) \;\in\; \mathcal{S}, \\ & \text{such that } \exists\, K > 0 \text{ with } \sum_{|j| > J} |c_j|^2 \leq \mathrm{e}^{-KJ}, \text{ for large } J \Bigg\}. \end{aligned} \tag{3.7}$$

Remark It is easy to check that the inequality in (3.7) is equivalent to the requirement that the coefficients of f satisfy

$$|c_j| \;\leq\; \mathrm{e}^{-K|j|},$$

for large $|j|$. Another equivalent definition of $\mathcal{C}$ is

$$\mathcal{C} \;=\; \cup_{t>0}\, \mathrm{e}^{-tH_{ho}}\, \mathcal{S},$$

where $H_{ho} \;=\; -\,\Delta/2 \,+\, x^2/2$ is the harmonic oscillator Hamiltonian. The set $\mathcal{C}$ is sometimes called the set of analytic vectors [17] for the harmonic oscillator Hamiltonian.

Theorem 3.6 *All theorems above remain true if the initial condition has the form*

$$\psi(x, 0, \hbar) = (\Lambda_\hbar(a, \eta) \varphi)(x),$$

where $\varphi \in \mathcal{C}$.

Theorem 3.1 is proved in Section 6. Theorem 3.2 is proved in Section 7. Theorems 3.3 and 3.4 are proved in Section 8. Theorem 3.5 is proved in Section 9. Theorem 3.6 is proved in Section 10.

4 An Alternative Semiclassical Expansion

In this section we derive an expansion in powers of $\hbar^{1/2}$. In later sections we perform optimal truncation of this expansion to obtain exponentially accurate approximations.

We wish approximately to solve the equation

$$i\hbar\,\frac{\partial\psi}{\partial t} \;=\; -\,\frac{\hbar^2}{2}\,\Delta\,\psi \,+\, V(x)\,\psi, \tag{4.1}$$

with initial conditions of the form

$$\psi(x,0,\hbar) \;=\; \sum_{|j|\le J} c_{0,j}(0)\,\phi_j(A(0),B(0),\hbar,a(0),\eta(0),x), \tag{4.2}$$

where $\sum\limits_{|j|\le J} |\,c_{0,j}(0)\,|^2 \;=\; 1.$

We can write the exact solution to this equation in the basis of semiclassical wave packets,

$$\psi(x,t,\hbar) \;=\; e^{iS(t)/\hbar}\,\sum_j c_j(t,\hbar)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x). \tag{4.3}$$

Note that the sum is over multi-indices j. The infinite vector c whose entries are the coefficients c_j satisfies

$$i\,\hbar\,\dot{c} \;=\; K(t,\hbar)\,c, \tag{4.4}$$

where $K(t,\hbar)$ is an infinite self–adjoint matrix.

The matrix $K(t,\hbar)$ has an asymptotic expansion in powers of $\hbar^{1/2}$. The cubic term in the expansion of $V(x)$ around $x = a(t)$ gives the leading non-zero term of order $\hbar^{3/2}$. The quartic term in the expansion of $V(x)$ gives the term of order $\hbar^{4/2}$, etc. Thus, we can write

$$K(t,\hbar) \;\sim\; \sum_{k=3}^{\infty} \hbar^{k/2}\,K_k(t), \tag{4.5}$$

with

$$K_k(t) \;=\; \sum_{|m|=k} \frac{(D^mV)(a(t))}{m!}\;X(t)^m, \tag{4.6}$$

where $X(t)^m$ is the infinite matrix that represents $\hbar^{-|m|/2}\,(x-a)^m$. Explicit formulas [10] show that entries of $X(t)^m$ and $K_k(t)$ do not depend on $\hbar$.

We formally expand the vector c as

$$\begin{aligned} c(t,\hbar) \;&=\; c_0(t) \,+\, \hbar^{1/2}\,c_1(t) \,+\, \hbar^{2/2}\,c_2(t) \,+\, \dots \\ &=\; \sum_k \hbar^{k/2}\,c_k(t). \end{aligned} \tag{4.7}$$

We denote the j^{th} entry of $c_k(t)$ by $c_{k,j}(t)$. Note that k is a non-negative integer, and j is a multi-index. We substitute the two expansions (4.5) and (4.7) into (4.4) and divide by $\hbar$. We then equate terms of the same orders on the two sides of the resulting equation.

Order 0**.** The zeroth order terms simply require

$$i\,\dot{c}_0 \;=\; 0. \tag{4.8}$$

From (4.2), the solution is obviously $c_{0,j}(t) \;=\; c_{0,j}(0)$. We note that $c_{0,j}(t) = 0$ if $|j| > J$.

Order 1**.** The first order terms require

$$i\,\dot{c}_1 \;=\; K_3(t)\,c_0(t). \tag{4.9}$$

We solve this by integrating. Because of (4.2), $c_1(0) \;=\; 0$. From the form of $c_0(t)$, only finitely many of the entries of $c_1(t)$ are non-zero, and $c_{1,j} \;=\; 0$ whenever $|j| > J+3$. In d space dimensions, $c_1(t)$ has at most $\begin{pmatrix} J+3+d \\ d \end{pmatrix}$ non-zero entries.

Order 2**.** The second order terms require

$$i\,\dot{c}_2 \;=\; K_4(t)\,c_0(t) \;+\; K_3(t)\,c_1(t). \tag{4.10}$$

Again, we can solve this by integrating with $c_2(0) \;=\; 0$. The only entries of $c_2(t)$ that can be non-zero are $c_{2,j}(t)$ with $|j| \le J+6$. In d dimensions, there are at most $\begin{pmatrix} J+6+d \\ d \end{pmatrix}$ non-zero entries.

Order n**.** In general, the n^{th} order terms require

$$i\,\dot{c}_n \;=\; \sum_{k=0}^{n-1} K_{n+2-k}(t)\,c_k(t). \tag{4.11}$$

To solve this, we simply integrate. We observe that $c_{n,j}(t)$ can be non-zero only if $|j| \le J+3n$. In d dimensions, there are at most $\begin{pmatrix} J+3n+d \\ d \end{pmatrix}$ non-zero entries.

Our expansion is different from the one constructed in [11], and it is different from the Dyson expansion used in [11]. All three of these expansions are asymptotic to the exact solution of the Schrödinger equation. We note that the main construction in [11] yields a normalized wave function. The expansion derived above does not generate normalized wavepackets.

To prove that this expansion is asymptotic, we apply Lemma 2.8 of [10]. To check the hypotheses of that lemma, we do the expansion above through order $(l-1)$ to obtain $c_0(t)$, $c_1(t)$, $\ldots$, $c_{l-1}(t)$. We substitute these into (4.7) with the sum cut off after $k = l-1$. We then use the result in (4.3) and compute

$$\xi_l(x,t,\hbar) \;=\; i\,\hbar\,\frac{\partial\psi}{\partial t}(x,t,\hbar) \;+\; \frac{\hbar^2}{2}\,\Delta\,\psi(x,t,\hbar) \;-\; V(x)\,\psi(x,t,\hbar) \tag{4.12}$$

Because the $c_k(t)$ solve (4.8), (4.9), (4.10), etc., there are many cancellations. We obtain

$$\xi_l(x,t,\hbar) \;=\; e^{iS(t)/\hbar}\,\sum_{k=0}^{l-1}\hbar^{k/2}\,W_{a(t)}^{(l+1-k)}(x)\sum_{|j|\le\widetilde{J}(l)} c_{k,j}(t)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x). \tag{4.13}$$

Here, $\widetilde{J}(l)=J+3l-3$, and for each q, $W_{a(t)}^{(q)}(x)$ denotes the Taylor series error

$$\begin{aligned} W_{a(t)}^{(q)}(x) &= V(x)\;-\;\sum_{|m|\le q}\frac{D^mV(a(t))}{m!}\,(x-a(t))^m \\ &= \sum_{|m|=q+1}\frac{D^mV(\zeta_m(x,a(t))}{m!}\,(x-a(t))^m, \end{aligned} \tag{4.14}$$

for some $\zeta_m(x,a(t))\;=\;a(t)+\theta_{m,x,a(t)}(x-a(t))$, with $\theta_{m,x,a(t)}\in(0,\,1)$.

If V is C^{l+2} on some neighborhood of $\{a(t)\,:\,t\in[0,T]\}$, then each $W_{a(t)}^{(q)}(x)$ that occurs in (4.13) is bounded on a slightly smaller neighborhood of $\{a(t)\,:\,t\in[0,T]\}$. Since $\|\,(x-a(t))^m\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)\,\|$ has order $\hbar^{|m|/2}$, it follows that $\|\,\xi(\cdot,t,\hbar)\,\|$ has order $\hbar^{l+2}$. Applying Lemma 2.8 of [10], we learn that the $\psi(x,t,\hbar)$ solves the Schrödinger equation up to an error whose norm is bounded by $C_l\,\hbar^{l/2}$, when $\hbar$ is sufficiently small.

Note that the argument above requires the insertion of cutoffs to handle the Gaussian tails or some other assumption, such as $V\in C^{l+2}(I\!R^d)$ with $|\,D^mV(x)\,|\;\le\;M_m\,\exp(\tau x^2)$ for $|m|\le l+2$.

5 Estimates of the Expansion Coefficients

In this section we study the behavior of $c_k(t)$.

The first step is to get a good estimate of the operator norm of the bounded operator $(x-a)^m\,P_{|j|\le n}$, where $P_{|j|\le n}$ denotes the projection onto the span of the ϕ_j with $|j|\le n$.

Lemma 5.1 *In d dimensions,*

$$(x-a)^m\,P_{|j|\le n}\;=\;P_{|j|\le n+|m|}\,(x-a)^m\,P_{|j|\le n}, \tag{5.1}$$

and

$$\|\,(x-a)^m\,P_{|j|\le n}\,\|\;\le\;\left(\sqrt{2\hbar}\;d\,\|\,A\,\|\right)^{|m|}\;\left(\frac{(n+|m|)!}{n!}\right)^{1/2}. \tag{5.2}$$

Proof: Formula (2.22) of [10] states that

$$(x_i-a_i)\;=\;\sqrt{\frac{\hbar}{2}}\;\left(\sum_p A_{i\,p}\,\mathcal{A}_p(A,B,\hbar,a,\eta)^*\;+\;\sum_p\overline{A_{i\,p}}\,\mathcal{A}_p(A,B,\hbar,a,\eta)\right).$$

Note that the right hand side contains $2d$ terms. Suppose v is any vector in the range of $P_{|j|\leq n}$. Then using formulas (2.8) and (2.9) of [10], we easily deduce that

$$\begin{aligned} \| \mathcal{A}_p(A,B,\hbar,a,\eta)^*\, v \| &\leq \sqrt{n+1}\; \| v \|, \\ \| \mathcal{A}_p(A,B,\hbar,a,\eta)\, v \| &\leq \sqrt{n}\; \| v \|, \end{aligned}$$

and that both $\mathcal{A}_p(A,B,\hbar,a,\eta)^*\, v$ and $\mathcal{A}_p(A,B,\hbar,a,\eta)\, v$ belong to the range of $P_{|j|\leq n+1}$.

It follows immediately that

$$\| \, (x_i - a_i)\, P_{|j|\leq n} \, \| \;\leq\; \sqrt{2\hbar}\; d\, \| \, A \, \| \, \sqrt{n+1},$$

and that $(x_i - a_i)\, P_{|j|\leq n} \;=\; P_{|j|\leq n+1}\, (x-a)\, P_{|j|\leq n}$.

The lemma follows from these two results by a simple induction. ■

The conclusion to the next lemma contains the binomial coefficients $\begin{pmatrix} k-1 \\ p-1 \end{pmatrix}$. For $k=1$ and $p=1$ we define this to be 1.

Lemma 5.2 *Suppose V satisfies the hypotheses of Theorem 3.1.*

Fix T and choose a classical orbit $a(t)$ for $0 \leq t \leq T$. The hypotheses guarantee that

$$D_1 \;=\; \max\; \left\{\; 1, \; \sup_{0\leq |n|,\; 0\leq t\leq T} \; \delta^{|n|}\; \frac{|\,(D^nV)(a(t))\,|}{n!} \;\right\} \tag{5.3}$$

and

$$D_2 \;=\; \max\; \left\{\; 1, \; \sup_{0\leq t\leq T} \; \sqrt{2}\; d\, \delta^{-1}\; \| \, A(t) \, \| \;\right\} \tag{5.4}$$

are finite.

We define $D_3 \;=\; \begin{pmatrix} d+2 \\ d-1 \end{pmatrix}$, which is the number of multi-indices m with $|m| = 3$ in d dimensions.

Suppose $c_0(0)$ is a normalized vector with $c_{0,j}(0)$ non-zero only for $|j| \leq J$, and suppose $c_{k,j}(0) \;=\; 0$ for all j when $k \geq 1$. Let $c_{k,j}(t)$ be the solution to (4.8), (4.9), ..., (4.11), with these initial conditions. Then for $t \in [0,\, T]$, we have

$$c_{0,j}(t) \;=\; 0 \qquad \textit{whenever} \qquad |j| > J, \tag{5.5}$$

$$\| \, c_0(t) \, \| \;\leq\; D_1, \tag{5.6}$$

and for $k \geq 1$,

$$c_k(t) \;=\; \sum_{p=1}^{k} \; c_k^{[p]}(t), \tag{5.7}$$

where

$$c_{k,j}^{[p]}(t) \;=\; 0 \qquad \textit{whenever} \qquad |j| > J+k+2p, \tag{5.8}$$

and

$$\| \, c_k^{[p]}(t) \, \| \;\leq\; \begin{pmatrix} k-1 \\ p-1 \end{pmatrix} \; D_1^p\, D_2^{k+2p}\, D_3^k \; \left(\frac{(J+k+2p)!}{J!} \right)^{1/2} \; \frac{t^p}{p!}. \tag{5.9}$$

Proof: The finiteness of D_1 and D_2 is standard.

The conclusions (5.5) and (5.6) are trivial.

We assume $t \in [0, T]$, and let $X(t)$ denote the formal vector whose entries $X_i(t)$ denote the infinite matrix that represents $\hbar^{-1/2}(x_i - a_i(t))$ in the basis $\{\,\phi_j(A(t), B(t), \hbar, a(t), \eta(t), \cdot)\,\}$.

From (4.9) we have

$$i\,\dot{c}_1(t) \;=\; K_3(t)\,c_0(t) \;=\; \sum_{|m|=3} \frac{(D^m V)(a(t))}{m!}\,X(t)^m\,c_0(t).$$

We integrate to obtain $c_1(t) \;=\; c_1^{[1]}(t)$. Lemma 5.1, (5.5), and (5.6) imply two conclusions:

$$c_{1,j}^{[1]}(t) \;=\; 0 \qquad \text{whenever} \qquad |j| > J+3, \tag{5.10}$$

and

$$\|\,c_1^{[1]}(t)\,\| \;\le\; D_1\,D_2^3\,D_3\,\left(\frac{(J+3)!}{J!}\right)^{1/2}\,t, \tag{5.11}$$

where the factor $\begin{pmatrix} d+2 \\ d-1 \end{pmatrix}$ is the number of multi-indices m with $|m| = 3$ in d dimensions. This proves (5.7), (5.8), and (5.9) for $k = 1$.

For $k = 2$, we have from (4.10),

$$\begin{aligned} i\,\dot{c}_2(t) \;&=\; K_4(t)\,c_0(t) \;+\; K_3(t)\,c_1(t) \\ &=\; \sum_{|m|=4} \frac{(D^m V)(a(t))}{m!}\,X(t)^m\,c_0(t) \;+\; \sum_{|m|=3} \frac{(D^m V)(a(t))}{m!}\,X(t)^m\,c_1(t). \end{aligned}$$

The two terms on the right hand side of this equation produce two terms, $c_2^{[1]}(t)$ and $c_2^{[2]}(t)$, when we integrate to obtain $c_2(t)$. Using (5.5), (5.6), (5.10), (5.11), and two applications of Lemma 5.1 we learn that $c_2(t) = c_2^{[1]}(t) \;+\; c_2^{[2]}(t)$, where

$$c_{2,j}^{[1]}(t) \;=\; 0 \qquad \text{whenever} \qquad |j| > J+4, \tag{5.12}$$

$$c_{2,j}^{[2]}(t) \;=\; 0 \qquad \text{whenever} \qquad |j| > J+6, \tag{5.13}$$

$$\|\,c_2^{[1]}(t)\,\| \;\le\; \begin{pmatrix} d+3 \\ d-1 \end{pmatrix}\,D_1\,D_2^4\,\left(\frac{(J+4)!}{J!}\right)^{1/2}\,t, \tag{5.14}$$

and

$$\|\,c_2^{[2]}(t)\,\| \;\le\; D_1^2\,D_2^6\,D_3^2\,\left(\frac{(J+6)!}{J!}\right)^{1/2}\,\frac{t^2}{2!}. \tag{5.15}$$

(The factor of $\begin{pmatrix} d+3 \\ d-1 \end{pmatrix}$ in (5.14) is the number of multi-indices m with $|m| = 4$.) This implies (5.7), (5.8), and (5.9) for $k = 2$ because $\begin{pmatrix} d+3 \\ d-1 \end{pmatrix} \leq \begin{pmatrix} d+2 \\ d-1 \end{pmatrix}^2 = D_3^2$. This combinatorial inequality follows because $d \geq 1$ implies

$$\begin{aligned}
\begin{pmatrix} d+2 \\ d-1 \end{pmatrix}^2 \begin{pmatrix} d+3 \\ d-1 \end{pmatrix}^{-1} &= \frac{(d+2)!^2\ 4!\ (d-1)!}{3!^2\ (d-1)!^2\ (d+3)!} \\
&= \frac{4d}{d+3}\ \frac{d+2}{3}\ \frac{d+1}{2} \ \geq\ \frac{4}{1+3/d} \ \geq\ 1. \qquad (5.16)
\end{aligned}$$

From (4.11) with $n = 3$, we have

$$\begin{aligned}
i\,\dot{c}_3(t) &= K_5(t)\,c_0(t) \ +\ K_4(t)\,c_1(t) \ +\ K_3(t)\,c_2(t) \\
&= \sum_{k=0}^{2}\ \sum_{|m|=5-k} \frac{(D^m V)(a(t))}{m!}\,X(t)^m\,c_k(t).
\end{aligned}$$

Using (5.5), (5.6), (5.10), (5.11), (5.12), (5.13), (5.14), (5.15), and four applications of Lemma 5.1 we learn that $c_3(t) = c_3^{[1]}(t) \ +\ c_3^{[2]}(t) \ +\ c_3^{[3]}(t)$, where

$$c_{3,j}^{[1]}(t) \ =\ 0 \qquad \text{whenever} \qquad |j| > J+5, \qquad (5.17)$$

$$c_{3,j}^{[2]}(t) \ =\ 0 \qquad \text{whenever} \qquad |j| > J+7, \qquad (5.18)$$

$$c_{3,j}^{[3]}(t) \ =\ 0 \qquad \text{whenever} \qquad |j| > J+9, \qquad (5.19)$$

$$\|\, c_3^{[1]}(t)\,\| \ \leq\ \begin{pmatrix} d+4 \\ d-1 \end{pmatrix} D_1\,D_2^5 \left(\frac{(J+5)!}{J!} \right)^{1/2} t, \qquad (5.20)$$

$$\|\, c_3^{[2]}(t)\,\| \ \leq\ \begin{pmatrix} d+3 \\ d-1 \end{pmatrix} 2\,D_1^2\,D_2^7\,D_3 \left(\frac{(J+7)!}{J!} \right)^{1/2} \frac{t^2}{2!}, \qquad (5.21)$$

and

$$\|\, c_3^{[3]}(t)\,\| \ \leq\ D_1^3\,D_2^9\,D_3^3 \left(\frac{(J+9)!}{J!} \right)^{1/2} \frac{t^3}{3!}. \qquad (5.22)$$

This implies (5.7), (5.8), and (5.9) for $k = 3$ because of (5.16) and the similar inequality

$$\begin{pmatrix} d+4 \\ d-1 \end{pmatrix} \ \leq\ \begin{pmatrix} d+2 \\ d-1 \end{pmatrix}^3 \ =\ D_3^3.$$

This inequality follows because $d \geq 1$ implies

$$\begin{pmatrix} d+2 \\ d-1 \end{pmatrix}^3 \begin{pmatrix} d+4 \\ d-1 \end{pmatrix}^{-1} \ =\ \frac{5}{1+4/d}\ \frac{4}{1+3/d} \left[\frac{d+2}{3}\ \frac{d+1}{2} \right]^2 \ \geq\ 1.$$

Now suppose inductively that the lemma is true for all $k \leq q$, for some $q \geq 2$. By integrating (4.11) with $n = q + 1$, we can decompose

$$c_{q+1}(t) \;=\; c_{q+1}^{[1]}(t) \,+\, \sum_{n=1}^{q} \sum_{p=2}^{n+1} d[q,n,p](t), \tag{5.23}$$

where

$$c_{q+1}^{[1]}(t) \;=\; -\,i \int_0^t K_{q+3}(s)\, c_0(s)\, ds, \tag{5.24}$$

$$d[q,n,p](t) \;=\; -\,i \int_0^t K_{q+3-n}(s)\, c_n^{[p-1]}(s)\, ds, \tag{5.25}$$

for $1 \leq n \leq q$ and $2 \leq p \leq n+1$. We interchange the sums in (5.23) to obtain

$$c_{q+1}(t) \;=\; c_{q+1}^{[1]}(t) \,+\, \sum_{p=2}^{q+1} c_{q+1}^{[p]}(t), \tag{5.26}$$

where

$$c_{q+1}^{[p]}(t) \;=\; \sum_{n=p-1}^{q} d[q,n,p](t), \tag{5.27}$$

for $2 \leq p \leq q+1$. This establishes (5.7) for $k = q+1$.

The induction hypotheses, formulas (4.6), (5.24), (5.25), (5.27), and Lemma 5.1 imply (5.8) for $k = q+1$, as well as the two inequalities

$$\|\, c_{q+1}^{[1]}(t) \,\| \;\leq\; \begin{pmatrix} d+q+2 \\ d-1 \end{pmatrix} D_1\, D_2^{q+3} \left(\frac{(J+q+3)!}{J!} \right)^{1/2} t, \tag{5.28}$$

and

$$\begin{aligned} \|\, d[q,n,p](t) \,\| \;&\leq\; \begin{pmatrix} d+q+2-n \\ d-1 \end{pmatrix} D_1\, D_2^{q+3-n} \left(\frac{(J+q+1+2p)!}{(J+n+2p-2!} \right)^{1/2} \\ &\quad \times \begin{pmatrix} n-1 \\ p-2 \end{pmatrix} D_1^{p-1}\, D_2^{n+2p-2}\, D_3^{n} \left(\frac{(J+n+2p-2)!}{J!} \right)^{1/2} \frac{t^p}{p!} \\ &= \begin{pmatrix} n-1 \\ p-2 \end{pmatrix} \begin{pmatrix} d+q+2-n \\ d-1 \end{pmatrix} D_1^{p}\, D_2^{q+2p+1}\, D_3^{n} \\ &\quad \times \left(\frac{(J+q+2p+1)!}{J!} \right)^{1/2} \frac{t^p}{p!}. \end{aligned} \tag{5.29}$$

From these inequalities and (5.26), we obtain (5.9) for $k = q+1$ as soon as we establish both the inequality

$$\begin{pmatrix} d+q+2-n \\ d-1 \end{pmatrix} \begin{pmatrix} d+2 \\ d-1 \end{pmatrix}^{n} \;\leq\; \begin{pmatrix} d+2 \\ d-1 \end{pmatrix}^{q+1} \tag{5.30}$$

for $0 \le n \le q$, and the identity

$$\binom{q}{p-1} = \sum_{n=p-1}^{q} \binom{n-1}{p-2}, \tag{5.31}$$

for $q \ge 2$ and $2 \le p \le q+1$.

We set $r = q - n$ and note that (5.30) is equivalent to

$$\binom{d+r+2}{d-1} \binom{d+2}{d-1}^{-r-1} \le 1, \tag{5.32}$$

for $0 \le r \le q$. However,

$$\begin{aligned} & \binom{d+r+2}{d-1} \binom{d+2}{d-1}^{-r-1} \\ = & \frac{(d+2+r)!}{(d-1)!\,(r+3)!} \left(\frac{(d-1)!\,3!}{(d+2)!} \right)^{r+1} \\ = & \left[\frac{r+4}{1} \left(\frac{1}{4}\right)^{r+1} \right] \left[\frac{r+5}{2} \left(\frac{2}{5}\right)^{r+1} \right] \cdots \left[\frac{r+d+2}{d-1} \left(\frac{d-1}{d+2}\right)^{r+1} \right]. \end{aligned}$$

Inequality (5.32) follows if each of the factors in the square brackets is bounded by 1. Thus, we need only prove

$$\frac{r+m+3}{m} \le \left(\frac{m+3}{m} \right)^{r+1},$$

for $1 \le m$, which can be verified by using the binomial expansion:

$$\frac{r+m+3}{m} = 1 + \frac{r+3}{m} \le 1 + (r+1)\frac{3}{m} + \cdots = \left(1 + \frac{3}{m}\right)^{r+1} = \left(\frac{m+3}{m} \right)^{r+1}.$$

This proves (5.32) and hence (5.30).

The identity (5.31) is trivial for $q = 2$ and $p = 2, 3$. Assume inductively that it is true for all $2 \le q \le m$ and $2 \le p \le q+1$, where $m \ge 2$. The identity (5.31) is trivial for $q = m+1$ and $p - 1 = m + 1$, since

$$\binom{m+1}{m+1} = 1 = \binom{m}{m}.$$

Then for $m + 1 > p - 1$, we have

$$\begin{aligned} \binom{m+1}{p-1} &= \frac{(m+1)!}{(p-1)!\,(m-p+2)!} \\ &= \frac{(p-1)\,(m!)}{(p-1)!\,(m-p+2)!} + \frac{(m-p+2)\,(m!)}{(p-1)!\,(m-p+2)!} \\ &= \binom{m}{p-2} + \binom{m}{p-1} \\ &= \binom{m}{p-2} + \sum_{n=p-1}^{m} \binom{n-1}{p-2} \\ &= \sum_{n=p-1}^{m+1} \binom{n-1}{p-2}. \end{aligned}$$

This proves (5.31) and completes the proof of the lemma. ∎

Corollary 5.3 *Assume the hypotheses of Lemma 5.2. Then in addition to (5.5) and (5.6), we have the following for $k \geq 1$:*

$$c_{k,j}(t) \;=\; 0, \qquad \textit{whenever} \qquad |j| > J + 3k, \tag{5.33}$$

and

$$\| \, c_k(t) \, \| \;\leq\; \left(\frac{(J+3k)!}{J!} \right)^{1/2} \; \frac{D_2^k \, D_3^k}{k!} \left(1 \,+\, D_1 \, D_2^2 \, t \right)^k . \tag{5.34}$$

Proof: Since $p \leq k$, (5.8) implies (5.33).

To prove (5.34), we note that $\dfrac{((J+k+2p)!)^{1/2}}{p!}$ is increasing in p. Thus, (5.9) and $p \leq k$ imply

$$\| \, c_k^{[p]}(t) \, \| \;\leq\; \begin{pmatrix} k-1 \\ p-1 \end{pmatrix} \; D_1^p \; D_2^{k+2p} \; D_3^k \; \left(\frac{(J+3k)!}{J!} \right)^{1/2} \; \frac{t^p}{k!}.$$

Summing over p, we obtain

$$\| \, c_k(t) \, \| \;\leq\; \left(\frac{(J+3k)!}{J!} \right)^{1/2} \; \frac{D_2^k \, D_3^k}{k!} \left(1 \,+\, D_1 \, D_2^2 \, t \right)^{k-1} \; D_1 \, D_2^2 \, t.$$

This implies (5.34). ∎

6 Optimal Truncation Estimates

In this section we show that the error given by (4.12) and (4.13) is exponentially small if we choose $l = [\![\, g/\hbar \,]\!]$ for an appropriate value of g.

The philosophy will be separately to estimate the error near the classical orbit and far from the orbit. To do so, we let b be any positive number and define $\chi_1(x,t)$ to be the characteristic function of $\{ \, x \,:\, |x - a(t)| \leq b \, \}$. We set $\chi_2(x,t) \;=\; 1 \,-\, \chi_1(x,t)$.

Lemma 6.1 *Assume V satisfies the hypotheses of Theorem 3.1. Define $\chi_1(x,t)$ as above and $\xi_l(x,t,\hbar)$ by (4.12). For fixed $T > 0$ and $b > 0$, there exists $G_1 > 0$, such that for each $g \in (0, G_1)$, there exist C_1 and $\gamma_1 > 0$, such that if l is chosen to depend on $\hbar$ as $l(\hbar) \;=\; [\![\, g/\hbar \,]\!]$, then*

$$\hbar^{-1} \int_0^T \| \, \chi_1(\cdot,t) \, \xi_{l(\hbar)}(\cdot,t,\hbar) \, \| \, dt \;\leq\; C_1 \, \exp\{ \, -\gamma_1/\hbar \, \} \, . \tag{6.1}$$

Proof: It is sufficient to prove the existence of α_1 and β_1, such that

$$\hbar^{-1} \int_0^T \| \, \chi_1(\cdot,t) \, \xi_l(\cdot,t,\hbar) \, \| \, dt \;\leq\; \alpha_1 \, \beta_1^l \, l^{l/2} \, \hbar^{l/2}. \tag{6.2}$$

If this can be established, we choose $G_1 = \beta_1^{-2}$. Then $0 < g < G_1$ and $l = [\![\, g/\hbar \,]\!]$ imply $\beta_1^2\, g \;=\; e^{-\omega}$, with $\omega > 0$. Since $\alpha_1\,(\beta_1^2\, l\, \hbar)^{l/2} \;=\; \alpha_1\, e^{-\omega g/(2\hbar)}$, this implies the lemma with $C_1 = \alpha_1$ and $\gamma_1 = \omega g/2$.

To prove (6.2), we note first that our hypotheses imply the finiteness of

$$D_4 \;=\; \sup_{|n|\geq 0,\ 0\leq t\leq T,\ |x-a(t)|\leq b} \delta^{|n|}\ \frac{|\,(D^nV)(x)\,|}{n!}. \tag{6.3}$$

We use this, (4.13), and (4.14) to see that

$$\begin{aligned}
&\|\,\chi_1(x,t)\,\xi_l(x,t,\hbar)\,\| \\
&\leq\ \left\|\ \sum_{k=0}^{l-1}\ \sum_{|m|=l+2-k} \hbar^{k/2}\ \chi_1(x,t)\ \frac{(D^mV)(\zeta_m(x,a(t))}{m!}\,(x-a(t))^m \right. \\
&\qquad\qquad \left. \times \sum_{|j|\leq \widetilde{J}(l)} c_{k,j}(t)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x) \right\| \\
&\leq\ \sum_{k=0}^{l-1} \hbar^{k/2}\, D_4\, \delta^{-l-2+k} \\
&\qquad \times \sum_{|m|=l+2-k} \left\|\,(x-a(t))^m \sum_{|j|\leq \widetilde{J}(l)} c_{k,j}(t)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x) \right\| \\
&\leq\ D_4\ \hbar^{l/2+1} \sum_{k=0}^{l-1} \delta^{-l-2+k} \sum_{|m|=l+2-k} \|\,X(t)^m\, c_k(t)\,\|,
\end{aligned}$$

where $X(t)$ is the infinite matrix that represents $\hbar^{-1/2}(x-a(t))$ in the ϕ_j basis.

Thus,

$$\hbar^{-1} \int_0^T \|\,\chi_1(\cdot,t)\,\xi_l(\cdot,t,\hbar)\,\|\,dt \ \leq\ D_4\,\hbar^{l/2} \sum_{k=0}^{l-1} \int_0^T \delta^{-l-2+k} \sum_{|m|=l+2-k} \|\,X(t)^m\,c_k(t)\,\|\,dt. \tag{6.4}$$

We apply Lemmas 5.1 and 5.2 to estimate each integral on the right hand side of (6.4). For $k=0$, we obtain

$$\begin{aligned}
\int_0^T \delta^{-l-2} \sum_{|m|=l+2} \|\,X(t)^m\,c_0(t)\,\|\,dt \ &\leq\ D_1\ D_2^{l+2} \begin{pmatrix} d+l+1 \\ d-1 \end{pmatrix} \left(\frac{(J+l+2)!}{J!}\right)^{1/2} T \\
&\leq\ \left(\frac{(J+3l)!}{J!}\right)^{1/2} \frac{D_2^{l+2}\,D_3^l}{(l-1)!}\ D_1\ D_2^2\ T.
\end{aligned} \tag{6.5}$$

In the last step, we have used $D_2 \geq 1$, (5.30), and $(J+l+2)! \;\leq\; \dfrac{(J+3l)!}{((l-1)!)^2}$, which is true for $l \geq 1$.

For $k \geq 1$, we write the integral on the right hand side of (6.4) as a sum of k terms by employing (5.7). By (5.8), (5.9), and Lemma 5.1, the p^{th} integrand satisfies

$$\begin{aligned}
&\delta^{-l-2+k} \sum_{|m|=l+2-k} \left\| \, X(t)^m \, c_k^{[p]}(t) \, \right\| \\
\leq \ & D_2^{l+2-k} \begin{pmatrix} d+l+1-k \\ d-1 \end{pmatrix} \left(\frac{(J+l+2p+2)!}{(J+k+2p)!} \right)^{1/2} \\
& \qquad \times \begin{pmatrix} k-1 \\ p-1 \end{pmatrix} D_1^p \, D_2^{k+2p} \, D_3^k \left(\frac{(J+k+2p)!}{J!} \right)^{1/2} \frac{t^p}{p!} \\
= \ & \begin{pmatrix} k-1 \\ p-1 \end{pmatrix} D_1^p \, D_2^{l+2p+2} \, D_3^k \begin{pmatrix} d+l+1-k \\ d-1 \end{pmatrix} \left(\frac{(J+l+2p+2)!}{J!} \right)^{1/2} \frac{t^p}{p!} \\
\leq \ & \begin{pmatrix} k-1 \\ p-1 \end{pmatrix} D_1^p \, D_2^{l+2p+2} \, D_3^l \left(\frac{(J+l+2p+2)!}{J!} \right)^{1/2} \frac{t^p}{p!}.
\end{aligned} \tag{6.6}$$

In the last step, we have again used (5.30).

We now mimic the proof of Corollary 5.3 and then integrate to obtain the following estimate of the k^{th} term in (6.4):

$$\left(\frac{(J+3l)!}{J!} \right)^{1/2} \frac{D_2^{l+2}}{(l-1)!} \, \frac{D_3^l}{(k+1) D_1 \, D_2^2} \left[\left(1 \, + \, D_1 \, D_2^2 \, T \right)^{k+1} \, - \, 1 \right].$$

We define

$$D_5 \ = \ 1 \, + \, D_1 \, D_2^2 \, T, \tag{6.7}$$

bound $\dfrac{D_3^l}{(k+1) D_1 \, D_2^2}$ by D_3^l, and $\left[(\, 1 \, + \, D_1 \, D_2^2 \, T \,)^{k+1} \, - \, 1 \right]$ by D_5^{k+1}. We then sum over k in (6.4) to obtain the estimate

$$\hbar^{-1} \int_0^T \| \, \chi_1(\cdot, t) \, \xi_l(\cdot, t, \hbar) \, \| \, dt \ \leq \ D_4 \, \hbar^{l/2} \left(\frac{(J+3l)!}{J!} \right)^{1/2} \frac{D_2^{l+2} \, D_3^l}{(l-1)!} \, \frac{D_5^{l+1}}{D_5 - 1}. \tag{6.8}$$

In this expression we bound $(J+3l)!$ by $(J+3l)^{J+3l}$ and $\dfrac{1}{(l-1)!}$ by $\dfrac{1}{\rho^{l-1} \, (l-1)^{l-1}}$, which holds for some constant ρ. After some algebra, this leads to the estimate (6.2). ■

To prove the analogous lemma with χ_1 replaced by χ_2, we use spherical coordinates for $\hbar^{-1/2}(x-a)$.

In spherical coordinates when $d \geq 2$, the operator $-\Delta_y \, + \, y^2$ has the form

$$- \, \frac{\partial^2}{\partial r^2} \ - \ \frac{d-1}{r} \, \frac{\partial}{\partial r} \ + \ \frac{\mathcal{L}^2}{r^2} \ + \ r^2.$$

Here $\mathcal{L}^2$ is the Laplace–Beltrami operator on S^{d-1}. For $d \geq 3$, it has eigenvalues

$$\lambda_q \ = \ q(q+d-2), \tag{6.9}$$

with multiplicities

$$\begin{aligned} m_q &= \frac{1}{(d-1)!}\,(q+1)\,(q+2)\,\cdots\,(q+d-3)\,\Big\{(q+d-2)(q+d-1)-(q-1)q\Big\} \\ &= \frac{1}{(d-2)!}\,(q+1)\,(q+2)\,\cdots\,(q+d-3)\;\;(d-1)(2q+d-2) \\ &\le C_d\; e^{\alpha_d q}, \end{aligned} \tag{6.10}$$

where $q = 0, 1, \ldots$. We denote a corresponding orthonormal basis of eigenfunctions by $Y_{q,m}(\omega)$ for $1 \le m \le m_q$.

When $d = 1$, the analog of the Laplace–Beltrami operator is multiplication by $\lambda = 0$ on even functions and multiplication by $\lambda = 1$ on odd functions. The operator $-\frac{\partial^2}{\partial x^2} + x^2$ on $I\!R$ just becomes the direct sum of two copies of $-\frac{\partial^2}{\partial r^2} + r^2$ on $(0, \infty)$ with Neumann and Dirichlet boundary conditions at $r = 0$.

When $d = 2$, (6.10) should be replaced with $m_0 = 1$ and $m_q = 2$ for $q > 0$, but the inequality $m_q \le C_d\, \mathrm{e}^{a_d q}$ still holds.

The eigenvalues of $-\Delta_y + y^2$ are $E = 4n + 2q + d$ with normalized eigenfunctions

$$\psi_{q,n,m}(r,\omega) \;=\; \sqrt{\frac{2n!}{\Gamma(q+n+\frac{d}{2})}}\;\; r^q\; L_n^{q+\frac{d}{2}-1}(r^2)\;\; e^{-r^2/2}\; Y_{q,m}(\omega). \tag{6.11}$$

Here

$$L_n^\beta(x) \;=\; \sum_{m=0}^{n}\,(-1)^m \begin{pmatrix} n+\beta \\ n-m \end{pmatrix} \frac{x^m}{m!} \tag{6.12}$$

denotes the Laguerre polynomial that satisfies the differential equation

$$x\,u''(x) \;+\; (\beta - x + 1)\,u'(x) \;+\; n\,u(x) \;=\; 0, \tag{6.13}$$

and the normalization condition

$$\int_0^\infty L_n^\beta(x)\; L_m^\beta(x)\; x^\beta\; e^{-x}\; dx \;=\; \begin{cases} 0 & \text{if } n \ne m \\ \frac{\Gamma(\beta+n+1)}{n!} & \text{if } n = m \end{cases}, \tag{6.14}$$

for $\beta > -1$.

The following lemma implies an estimate for $|\psi_{q,n,m}(r,\omega)|$ when r is in the region which is classically forbidden because of energy considerations.

Lemma 6.2 *For $\beta = q + \frac{d}{2} - 1$ with $q = 0, 1, \ldots$, the Laguerre polynomial $L_n^\beta(x)$ in (6.11) satisfies $|L_n^\beta(x)| \;\le\; \frac{x^n}{n!}$ whenever $x \;>\; 4n + 2\beta + 2 \;=\; 4n + 2q + d$.*

Proof: We mimic the proof of Lemma 3.1 of [11]. The first step is to show that $g(r) = r^\beta\; L_n^\beta(r^2)\;\; e^{-r^2/2}$ cannot vanish in the classically forbidden region $r^2 \;>\; 4n + 2q + d$. This function vanishes at infinity and is a non-trivial solution to an equation of the form

$$-\,g''(r) \;+\; w(r)\,g(r) \;=\; 0,$$

where $w(r) > 0$ for $r^2 > 4n + 2q + d$. From this differential equation we conclude that g and g'' have the same sign in this region. By standard uniqueness theorems, g and g' cannot both vanish at the same point. To obtain a contradition, suppose g has a zero at some point r_1 with $r_1^2 > 4n + 2q + d$. Since g vanishes at infinity, the mean value theorem guarantees that $g'(r_2) = 0$ for some $r_2 > r_1$. Without loss of generality, we may assume $g(r_2) > 0$. This forces $g''(r_2) > 0$, so g' is locally increasing. It follows that g' is increasing for all $r > r_2$. Thus, g could not go to zero at infinity. This contradiction shows that g could not have had a zero in the region.

We now proceed by induction on n. Since $L_0^\beta(x) = 1$, the lemma is true for $n = 0$. We now assume $n \geq 1$ and that the lemma has been established for $L_{n-1}^\beta(x)$.

Our non-vanishing result and (6.12) imply

$$\frac{L_n^\beta(x)\ n!}{(-1)^n\ x^n} \;=\; 1 \;-\; B_{\beta,n}(x),$$

where $B_{\beta,n}(x) = O(1/x)$ for large x, and $B_{\beta,n}(x) > -1$, for $x > 4n + 2\beta + 2$.

Using recurrence relation 8.971.3 of [6], we have

$$\begin{aligned} \frac{d}{dx}\,B_{\beta,n}(x) \;&=\; \frac{x\,L_n^{\beta\,\prime}(x) \;-\; n\,L_n^\beta(x)}{x^{n+1}}\;\frac{n!}{(-1)^n} \\ &=\; -\;\frac{(n+\beta)\,L_{n-1}^\beta(x)}{x^{n+1}}\;\frac{n!}{(-1)^n}. \end{aligned}$$

By our induction hypothesis, $L_{n-1}^\beta(x)$ has sign $(-1)^{n-1}$ for $x > 4n + 2\beta - 2$, which includes the region of interest.

Thus, $B_{\beta,n}(x)$ is increasing. Since it goes to zero at infinity, it cannot be positive. This implies the lemma. ∎

Lemma 6.3 *Assume V satisfies the hypotheses of Theorem 3.1. Define $\chi_2(x,t)$ as above and $\xi_l(x,t,\hbar)$ by (4.12). For fixed $T > 0$ and $b > 0$, there exists $G_2 > 0$, such that for each $g \in (0,\, G_2)$, there exist C_2 and $\gamma_2 > 0$, such that if l is chosen to depend on $\hbar$ as $l(\hbar) = [\![\, g/\hbar \,]\!]$, and $\hbar$ is sufficiently small, then*

$$\hbar^{-1}\,\int_0^T \|\,\chi_2(\cdot,t)\,\xi_{l(\hbar)}(\cdot,t,\hbar)\,\|\,dt \;\leq\; C_2\,\exp\{\,-\gamma_2/\hbar\,\}\,. \tag{6.15}$$

Proof: We begin by using the analyticity of V to control Taylor series errors. We define

$$C_\delta(x) = \{z \in \mathbb{C}^d \;:\; z_j = x_j + \delta e^{i\theta_j},\ \theta_j \in [0, 2\pi),\ j = 1, 2, \cdots, d\}.$$

If $z \in C_\delta(\zeta(x,a))$, then, for all $j = 1, 2, \cdots, d$,

$$|z_j| \;\leq\; \delta + |\zeta_j(x,a)| \;\leq\; \delta + |a_j| + |x_j - a_j|.$$

Using this and applying $(b+c)^2 \leq 2(b^2+c^2)$ several times, we see that $z \in C_\delta(\zeta(x,a))$ implies

$$|\,V(z)\,| \;\leq\; M\,\exp(2\tau(x-a)^2)\,\exp(4\tau(\delta^2 d + a^2)).$$

Hence, writing $\frac{1}{m!}\,D^m V(\zeta(x,a))$ as a d–dimensional Cauchy integral, we obtain the bound

$$\frac{1}{p!}\,|D^p V(\zeta(x,a))| \;\leq\; M\,\frac{\exp(4\tau(\delta^2 d + a^2))}{\delta^{|p|}}\;\exp(2\tau(x-a)^2),$$

where $\zeta(x,a)$ is any value between x and a. Thus, for $0 \leq t \leq T$, there exists a constant M_1, such that

$$\frac{1}{p!}\,|(D^p V)(\zeta_p(x,a(t)))| \;\leq\; \frac{M_1}{\delta^{|p|}}\;\exp(2\tau(x-a(t))^2). \tag{6.16}$$

We use this, (4.13), (4.14), and (5.33) to see that

$$\begin{aligned}
&\|\,\chi_2(x,t)\,\xi_l(x,t,\hbar)\,\| \\
&\leq\; \left\|\,\sum_{k=0}^{l-1}\hbar^{k/2}\,\chi_2(x,t)\sum_{|p|=l+2-k}\frac{(D^pV)(\zeta_p(x,a(t))}{p!}\,(x-a(t))^p\right. \\
&\qquad\qquad \left.\times\sum_{|j|\leq J+3k}c_{k,j}(t)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)\right\| \\
&\leq\; \sum_{k=0}^{l-1}\hbar^{k/2}\,M_1\,\delta^{-l-2+k}\sum_{|p|=l+2-k}\left\|\,\chi_2(x,t)\,\exp(2\tau(x-a(t))^2)\,(x-a(t))^p\right. \\
&\qquad\qquad \left.\times\sum_{|j|\leq J+3k}c_{k,j}(t)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)\right\| \\
&\leq\; M_1\,\delta^{-l-2}\sum_{k=0}^{l-1}\hbar^{k/2}\,\delta^k\sum_{|j|\leq J+3k}|c_{k,j}(t)|\sum_{|p|=l+2-k}\left\|\,\chi_2(x,t)\,e^{2\tau(x-a(t))^2}\,(x-a(t))^p\right. \\
&\qquad\qquad \left.\times\quad\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)\right\|.
\end{aligned} \tag{6.17}$$

Note that (5.33) has been used to replace $|j| \leq \widetilde{J}(l)$ with $|j| \leq J+3k$.

The norm in the final expression of (6.17) equals

$$\left\|\,\chi_{\{\,z:\,|z|>b\,\}}(x)\,\exp(2\tau x^2)\,x^p\,\phi_j(A(t),B(t),\hbar,0,0,x)\,\right\|, \tag{6.18}$$

where $|p| = l+2-k$.

We assume that $\hbar$ is sufficiently small that $4\tau\hbar|A(t)|^2 \,<\, 2/3$. Then the square of the quantity (6.18) equals

$$\begin{aligned}
&2^{-|j|}\,(j!)^{-1}\,\pi^{-d/2}\,|\det\,A(t)|^{-1}\,\hbar^{-d/2} \\
&\qquad\qquad\times\;\int_{|x|>b}x^{2p}e^{4\tau x^2}\,|\mathcal{H}_j(A;\,|A(t)|^{-1}\,\hbar^{-1/2}x)|^2\,e^{-|A(t)|^{-2}x^2/\hbar}\,dx \\
&\leq\;\frac{(\hbar\,\|A(t)\|^2)^{|p|}}{2^{|j|}\,(j!)\,\pi^{d/2}}\;\int_{\hbar^{1/2}|\,|A(t)|\,y\,|>b}|y|^{2|p|}\,|\mathcal{H}_j(A;\,y)|^2\,e^{(4\tau\hbar|A(t)|^2-1)y^2}\,dy.
\end{aligned}$$

$$\leq \quad \frac{(\hbar\,\|A(t)\|^2)^{|p|}}{2^{|j|}\,(j!)\,\pi^{d/2}}\;\int_{\hbar^{1/2}|\,|A(t)|\,y\,|>b}|y|^{2|p|}\,|\mathcal{H}_j(A;\,y)|^2\,e^{-y^2 2/3}\,dy$$

$$\leq \quad \mathrm{e}^{-b^2/(6\|A(t)\|^2\hbar)}\,\frac{(\hbar\,\|A(t)\|^2)^{|p|}}{2^{|j|}\,(j!)\,\pi^{d/2}}\;\int_{\hbar^{1/2}|\,|A(t)|\,y\,|>b}|y|^{2|p|}\,|\mathcal{H}_j(A;\,y)|^2\,e^{-y^2 1/2}\,dy. \tag{6.19}$$

By formula (3.7) of [11], $\Omega_j(y) \;=\; \sqrt{\frac{1}{2^{|j|}\,j!\,\pi^{d/2}}}\;\mathcal{H}_j(A;\,y)\;e^{-y^2/2}$ is a normalized eigenfunction of $-\Delta_y \,+\, y^2$ with eigenvalue $2|j|+d$. Thus, in spherical coordinates, it can be written as

$$\Omega_j(y) \;=\; \sum_{\{q,n,m:\,2n+q=|j|\}} d_{j,q,n,m}\,\psi_{q,n,m}(r,\omega), \tag{6.20}$$

where $\displaystyle\sum_{\{q,n,m:\,2n+q=|j|\}} |d_{j,q,n,m}|^2 \;=\; 1.$

We ultimately choose $l \,=\, [\![\, g/\hbar\,]\!]$, with $0<g<G_2$. Since $\widetilde{J}(l) \,=\, J+3l-3$, there exists C_3, such that $\hbar<1$ implies $\widetilde{J}(l) \leq C_3/\hbar$. By choosing G_2 sufficiently small, we also have $\widetilde{J}(l) \,<\, (\|A(t)\|^{-2}b^2-1)/(2\hbar)$ for $0\leq t\leq T$ and small $\hbar$. Thus, the relevant values of j in (6.19) satisfy $\sqrt{2|j|+d} \,<\, \|A(t)\|^{-1}b\hbar^{-1/2}$.

Lemma 6.2 shows that $\left|\,r^q\,L_n^{q+\frac{d}{2}-1}(r^2)\,\right| \;\leq\; \dfrac{r^{2n+q}}{n!}$ whenever $r^2 \;>\; 4n+2q+d=2|j|+d$. So, we see that (6.19) is bounded by

$$\hbar^{|p|}\,\|A(t)\|^{2|p|}\int_{S^{d-1}}\int_{r>\frac{b}{\|A\|\hbar^{1/2}}} r^{2|p|}\left|\sum_{\{q,n,m:\,2n+q=|j|\}} d_{j,q,n,m}\psi_{q,n,m}(r,\omega)\right|^2 e^{r^2/2}\,r^{d-1}dr\,d\omega.$$

We interchange the sum and integrals and apply the Schwartz inequality to the sum. This shows that (6.19) is bounded by

$$\begin{aligned}
&\mathrm{e}^{-b^2/(6\|A(t)\|^2\hbar)}\,\hbar^{|p|}\,\|A(t)\|^{2|p|}\sum_{\{q,n,m:\,2n+q=|j|\}}\frac{2n!}{\Gamma(q+\frac{d}{2}+n)}\\
&\qquad\times\;\int_{\frac{b}{\|A\|\hbar^{1/2}}}^{\infty} r^{d-1+2|p|+2q}\left|L_n^{q+\frac{d}{2}-1}(r^2)\right|^2 e^{-r^2/2}\,dr\int_{S^{d-1}}|\,Y_{q,m}(\omega)\,|^2\,d\omega\\
&=\;\mathrm{e}^{-b^2/(6\|A(t)\|^2\hbar)}\,\hbar^{|p|}\,\|A(t)\|^{2|p|}\sum_{\{q,n,m:\,2n+q=|j|\}}\frac{2n!}{\Gamma(q+\frac{d}{2}+n)}\\
&\qquad\qquad\times\;\int_{\frac{b}{\|A\|\hbar^{1/2}}}^{\infty} r^{d-1+2|p|+2q}\left|L_n^{q+\frac{d}{2}-1}(r^2)\right|^2 e^{-r^2/2}\,dr.
\end{aligned} \tag{6.21}$$

By reducing the value of G_2 if necessary, we can ensure that the hypotheses of Lemma 6.2 are satisfied in the integration region in the right hand side of (6.21). So, Lemma 6.2 shows that the integral satisfies

$$
\begin{aligned}
&\int_{\frac{b}{\|A\|\hbar^{1/2}}}^{\infty} r^{d-1+2|p|+2q}\left|L_n^{q+\frac{d}{2}-1}(r^2)\right|^2 e^{-r^2/2}\,dr\\
\leq\ & \frac{1}{(n!)^2}\int_{\frac{b}{\|A\|\hbar^{1/2}}}^{\infty} r^{4n+d-1+2|p|+2q}\,e^{-r^2/2}\,dr\\
\leq\ & \frac{2^{2n+\frac{d}{2}+q+|p|}}{(n!)^2}\int_0^{\infty} z^{4n+d-1+2q+2|p|}\,e^{-z^2}\,dz\\
=\ & \frac{2^{2n+\frac{d}{2}+q+|p|-1}}{(n!)^2}\,\Gamma(2n+\frac{d}{2}+q+|p|).
\end{aligned}
$$

So, (6.21) is bounded by

$$
\mathrm{e}^{-b^2/(6\|A(t)\|^2\hbar)}\hbar^{|p|}\,\|A(t)\|^{2|p|}\sum_{\{q,n,m:\,2n+q=|j|\}}\frac{2^{2n+\frac{d}{2}+q+|p|}}{n!}\,\frac{\Gamma(2n+\frac{d}{2}+q+|p|)}{\Gamma(q+\frac{d}{2}+n)}.
$$

We use (6.10) to estimate the sum over $m\leq m_q$ and bound this by

$$
\begin{aligned}
&C_d\,\mathrm{e}^{-b^2/(6\|A(t)\|^2\hbar)}\,\hbar^{|p|}\,\|A(t)\|^{2|p|}\sum_{\{n,q:\,q=|j|-2n\}} e^{\alpha_d q}\,\frac{2^{|j|+\frac{d}{2}+|p|}}{n!}\,\frac{\Gamma(|j|+\frac{d}{2}+|p|)}{\Gamma(q+\frac{d}{2}+n)}\\
=\ & C_d\mathrm{e}^{-b^2/(6\|A(t)\|^2\hbar)}\,\hbar^{|p|}\,\|A(t)\|^{2|p|}\,2^{|j|+\frac{d}{2}+|p|}\,e^{\alpha_d|j|}\,\Gamma(|j|+\frac{d}{2}+|p|)\\
&\qquad\qquad\times\sum_{n\leq|j|/2}\frac{e^{-2\alpha_d n}}{n!\;\Gamma(q+\frac{d}{2}+n)}.
\end{aligned}
$$

Since $e^{-2\alpha_d n}\leq 1$, this is bounded by

$$
C_d'\,\mathrm{e}^{-b^2/(6\|A(t)\|^2\hbar)}\,\hbar^{|p|}\,\|A(t)\|^{2|p|}\,2^{|j|+|p|}\,e^{\alpha_d|j|}\,\Gamma(|j|+\frac{d}{2}+|p|)\sum_{n\leq|j|/2}\frac{1}{n!\,\Gamma(q+\frac{d}{2}+n)}.
\tag{6.22}
$$

For $n\leq|j|/2$ and d fixed, there exists a constant C'', such that $\Gamma(|j|-n+\dfrac{d}{2})\;\geq\;C''\,(|j|-n)!$. So, the sum over n in (6.22) is bounded by

$$
\frac{1}{C''}\sum_{n\leq|j|/2}\frac{1}{n!\,(|j|-n)!}\;\leq\;\frac{1}{C''\,|j|!}\sum_{n\leq|j|/2}\binom{|j|}{n}\;\leq\;C'''\,\frac{2^{|j|}}{|j|!}.
$$

Thus, (6.21) is bounded by

$$
C''''\,\mathrm{e}^{-b^2/(6\|A(t)\|^2\hbar)}\,\hbar^{|p|}\,\|A(t)\|^{2|p|}\,2^{|p|}\,e^{\beta_d|j|}\,\frac{\Gamma(|j|+\frac{d}{2}+|p|)}{|j|!}.
\tag{6.23}
$$

This quantity bounds (6.19), which, in turn, bounds the square of (6.18). Terms of the form (6.18) occur in (6.17). Putting this all together, we see that (6.17) is bounded by

$$M_1\,C''''^{1/2}\,\mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)}\,\delta^{-l-2}\,\sum_{k=0}^{l-1}\,\hbar^{k/2}\,\delta^k\sum_{|j|\le J+3k}\frac{|c_{k,j}(t)|}{\sqrt{|j|!}}\,e^{\beta_d|j|/2}$$

$$\times\qquad\sum_{|p|=l+2-k}\hbar^{|p|/2}\,\|A(t)\|^{|p|}\,2^{|p|/2}\sqrt{\Gamma(|j|+\frac{d}{2}+|p|)}\,. \tag{6.24}$$

The number of terms that occur in the final sum of this expression is $\begin{pmatrix} l-k+d+1\\ d-1\end{pmatrix}$, and the terms in that sum are increasing. Thus, (6.24) is bounded by

$$\begin{aligned}
&M_1\,C''''^{1/2}\,\mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)}\,\delta^{-l-2}\,\sum_{k=0}^{l-1}\,\hbar^{k/2}\,\delta^k\sum_{|j|\le J+3k}\frac{|c_{k,j}(t)|}{\sqrt{|j|!}}\,e^{\beta_d|j|/2}\\
&\times\qquad\begin{pmatrix} l-k+d+1\\ d-1\end{pmatrix}\left(2\,\hbar\,\|A(t)\|^2\right)^{(l+2-k)/2}\sqrt{\Gamma(|j|+\frac{d}{2}+l+2-k)}\\
=\;&M_1\,C''''^{1/2}\,\mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)}\,\delta^{-l-2}\,\left(2\,\hbar\,\|A(t)\|^2\right)^{\frac{l}{2}+1}\sum_{k=0}^{l-1}\delta^k\,\left(2\,\|A(t)\|^2\right)^{-k/2}\\
&\times\qquad\begin{pmatrix} l-k+d+1\\ d-1\end{pmatrix}\sum_{|j|\le J+3k}\frac{|c_{k,j}(t)|}{\sqrt{|j|!}}\,e^{\beta_d|j|/2}\sqrt{\Gamma(|j|+\frac{d}{2}+l+2-k)}\,.
\end{aligned}$$

Applying the Schwartz inequality to the sum over j, we see that this expression is bounded by

$$M_1\,C''''^{1/2}\,\mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)}\,\delta^{-l-2}\,\left(2\,\hbar\,\|A(t)\|^2\right)^{\frac{l}{2}+1}\sum_{k=0}^{l-1}\delta^k\,\left(2\,\|A(t)\|^2\right)^{-k/2}$$

$$\times\qquad\begin{pmatrix} l-k+d+1\\ d-1\end{pmatrix}\|c_k(t)\|\left(\sum_{|j|\le J+3k}\frac{e^{\beta_d|j|}}{|j|!}\,\Gamma(|j|+\frac{d}{2}+l+2-k)\right)^{1/2}.$$

The number of terms that occur in the final sum of this expression is $\begin{pmatrix} J+3k+d\\ d\end{pmatrix}$, and the terms in that sum are increasing. Thus, the expression is bounded by

$$M_1\,C''''^{1/2}\,\mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)}\,\delta^{-l-2}\,\left(2\,\hbar\,\|A(t)\|^2\right)^{\frac{l}{2}+1}\sum_{k=0}^{l-1}\delta^k\,\left(2\,\|A(t)\|^2\right)^{-k/2}$$

$$\times\begin{pmatrix} l-k+d+1\\ d-1\end{pmatrix}\|c_k(t)\|\left[\begin{pmatrix} J+3k+d\\ d\end{pmatrix}\frac{e^{\beta_d(J+3k)}}{(J+3k)!}\Gamma(J+2k+\frac{d}{2}+l+2)\right]^{1/2}.$$

We now apply the estimate of $\|c_k(t)\|$ from Corollary 5.3 to bound this by

$$M_1\,C''''^{1/2}\,\mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)}\delta^{-l-2}\,\left(2\,\hbar\,\|A(t)\|^2\right)^{\frac{l}{2}+1}$$

$$
\begin{aligned}
&\times \quad \sum_{k=0}^{l-1} \delta^k \left(2\,\|A(t)\|^2\right)^{-k/2} \begin{pmatrix} l-k+d+1 \\ d-1 \end{pmatrix} \begin{pmatrix} J+3k+d \\ d \end{pmatrix}^{1/2} \\
&\qquad \times \quad e^{\beta_d(J+3k)/2}\, \frac{D_2^k D_3^k (1+D_1D_2^2|t|)^k}{k!} \left(\frac{\Gamma(J+2k+\frac{d}{2}+l+2)}{J!}\right)^{1/2} \\
\leq \quad & M_1 C''''^{1/2} \mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)} \delta^{-l-2} \left(2\,\hbar\,\|A(t)\|^2\right)^{\frac{l}{2}+1} \frac{e^{\beta_d J/2}}{\sqrt{J!}} \\
&\times \quad \sum_{k=0}^{l-1} \delta^k \left(2\,\|A(t)\|^2\right)^{-k/2} \begin{pmatrix} l-k+d+1 \\ d-1 \end{pmatrix} \begin{pmatrix} J+3k+d \\ d \end{pmatrix}^{1/2} \\
&\qquad\qquad \times \quad e^{3\beta_d k/2}\, \frac{D_2^k D_3^k (1+D_1D_2^2|t|)^k}{k!} \sqrt{\Gamma(J+2k+\frac{d}{2}+l+2)}.
\end{aligned} \tag{6.25}
$$

We now employ the following inequalities that hold for some numbers D_5 and D_6:

$$
\begin{aligned}
\begin{pmatrix} l-k+d+1 \\ d-1 \end{pmatrix} &\leq \begin{pmatrix} l+d+1 \\ d-1 \end{pmatrix}, \\
\begin{pmatrix} J+3k+d \\ d \end{pmatrix} &\leq \begin{pmatrix} J+3l-3+d \\ d \end{pmatrix}, \\
e^{3\beta_d k/4} &\leq e^{3\beta_d (l-1)/4}, \\
D_2^k\, D_3^k\, (1+D_1D_2^2|t|)^k &\leq D_5^{l-1}, \\
\frac{1}{k!}\sqrt{\Gamma(J+2k+\frac{d}{2}+l+2)} &\leq \frac{1}{(l-1)!}\sqrt{\Gamma(J+3l+\frac{d}{2})}, \qquad \text{and} \\
\sum_{k=0}^{l-1} \delta^k \left(2\,\|A(t)\|^2\right)^{-k/2} &\leq D_6^l.
\end{aligned}
$$

We then see that (6.25) is bounded by

$$
\begin{aligned}
& M_1 C''''^{1/2} \mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)}\, \delta^{-l-2} \left(2\,\hbar\,\|A(t)\|^2\right)^{\frac{l}{2}+1} \frac{e^{\beta_d J/2}}{\sqrt{J!}} \begin{pmatrix} l+d+1 \\ d-1 \end{pmatrix} \\
&\times \quad \begin{pmatrix} J+3l-3+d \\ d \end{pmatrix}^{1/2} \mathrm{e}^{3\beta_d(l-1)/4}\, D_5^{l-1}\, D_6^l\, \frac{1}{(l-1)!} \sqrt{\Gamma(J+3l+\frac{d}{2})}.
\end{aligned} \tag{6.26}
$$

We bound this expression by using the two inequalities

$$
\begin{aligned}
\begin{pmatrix} l+d+1 \\ d-1 \end{pmatrix} &\leq (l+d+1)^{d-1} \qquad \text{and} \\
\begin{pmatrix} J+3l-3+d \\ d \end{pmatrix} &\leq (J+3l-3+d)^d.
\end{aligned}
$$

Note that the right hand sides of these inequalities grow polynomially with l.

Since d is fixed, we conclude that (6.26), and hence, (6.17) are bounded by a constant times

$$\mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)}\ \frac{\mathrm{e}^{\gamma' J}}{\sqrt{J!}}\,\hbar^{l/2}\ \frac{\mathrm{e}^{\gamma l}}{(l-1)!}\ \sqrt{\Gamma(J+3l+\frac{d}{2})}, \tag{6.27}$$

for some positive γ, and γ'. With J fixed, we apply Stirling's formula to the factorial and Γ function to bound this by another constant times

$$\mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)}\ \hbar^{l/2}\ e^{\gamma l}\ \frac{(3l)^{3l/2}}{l^l}\ =\ \left(e^{\gamma}\,3^{3/2}\right)^l\ (\hbar\,l)^{l/2+1}.$$

By choosing $l\ =\ [\![\,g/\hbar\,]\!]$ for some sufficiently small $g>0$, this is bounded by a constant times $e^{-\gamma_2/\hbar}$.

This implies the lemma. ■

Theorem 3.1 follows immediately from Lemmas (6.1) and (6.3) with $G\ =\ \min\{\,G_1,\ G_2\,\}$.

7 Localization Estimates for the Wave Packets

In this section we show that our wave packets are localized near the classical path. Given any $\epsilon>0$, we can choose the truncation parameter $g>0$, such that our exponentially accurate wave packet is concentrated within $\{\,x\,:\,|x-a(t)|<b\,\}$ up to an exponentially small error.

Proof of Theorem 3.2: Let $\chi(x,t)$ be the characteristic function of the set $\{\,x\,:\,|x-a(t)|>b\,\}$, and let $\psi(x,t,\hbar)$ be the result of our construction with the series truncated with $l(\hbar)\ =\ [\![\,g/\hbar\,]\!]$.

We must prove

$$\|\,\chi(\cdot,t)\,\psi(\cdot,t,\hbar)\,\|\ \le\ \exp\{\,-\Gamma/\hbar\,\}, \tag{7.1}$$

for some $\Gamma>0$ when $g>0$ is sufficiently small.

The left hand side of (7.1) is bounded by

$$\sum_{k=0}^{l-1}\ \sum_{|j|\le J+3k}\ |c_{k,j}(t)|\ \|\,\chi(\cdot,t)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),\cdot)\,\|. \tag{7.2}$$

The norm in this sum has the form (6.18), with $n=0$ and $\tau=0$. Mimicking the estimation of (6.18), we obtain the estimate that corresponds to (6.24). We conclude that if $g>0$ is sufficiently small, then

$$\|\,\chi(\cdot,t)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),\cdot)\,\|\ \le\ \mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)}\ \mathrm{e}^{|j|\tilde{\beta}_d}$$

whenever $|j|\le J+3l(\hbar)-3$, for some $\tilde{\beta}_d$.

We use this and the Schwarz inequality to obtain, for some constants C_0, C_1, C_2 and C_3

$$\sum_{k=0}^{l-1} \sum_{|j|\leq J+3k} \hbar^{k/2} \, |c_{k,j}(t)| \, \| \, \chi(\cdot,t) \, \phi_j(A(t),B(t),\hbar,a(t),\eta(t),\cdot) \, \|$$

$$\leq \sum_{k=0}^{l-1} \hbar^{k/2} \, \| \, c_k(t) \, \| \, \mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)} \left(\sum_{|j|\leq J+3k} \mathrm{e}^{|j|2\tilde{\beta}_d} \right)^{1/2}$$

$$\leq \mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)} D_1 D_2^2 t \sum_{k=0}^{l-1} \hbar^{k/2} \left(\frac{(J+3k)!}{J!} \right)^{1/2} \frac{C_0^k D_5^k}{k!} \, \mathrm{e}^{\tilde{\beta}_d J} (J+3k+d)^{d/2} \tag{7.3}$$

$$\leq \mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)} \, C_1 \sum_{k=0}^{\infty} (\hbar C_2 k)^{k/2} \ \leq \ C_3 \, \mathrm{e}^{-b^2/(12\|A(t)\|^2\hbar)}, \tag{7.4}$$

provided g is small enough that $\hbar \, C_2 \, k \ \leq \ C_2 \, g \ < \ 1$ is satisfied. ■

8 Ehrenfest Time Scale

In this section we consider the accuracy of our construction when we allow T to grow as $\hbar \to 0$. Since the results stated in Theorem 3.4 and the method of proof are basically equivalent to those of [11], we will be rather sketchy.

Proof of Theorem 3.3: The first point to notice is that the since potential is bounded from below, energy conservation implies that $a(t)$ grows at most linearly with time. The exponential bound on the potential then implies the existence of $\widetilde{D}_1 > 0$ and $v > 0$ such that the quantity (5.3) is bounded by

$$D_1(T) \ \leq \ \widetilde{D}_1 \, \mathrm{e}^{v\tau T}.$$

Similarly, the existence of the Lyapunov exponent λ implies the existence of $\widetilde{D}_2$ such that the quantity (5.4) satisfies

$$D_2(T) \ \leq \ \tilde{D}_1 \, \mathrm{e}^{\lambda T}.$$

It then remains for us to keep track of the time dependence in the proof of Theorem 3.1. In particular, the quantities (6.3) and (6.7) fulfill the following estimates, modulo a possible increase of v:

$$\begin{aligned} D_4(T) \ &\leq \ D_1(T), \\ D_5(T) \ &\leq \ \widetilde{D}_5 \, \mathrm{e}^{(v\tau+2\lambda)T}. \end{aligned}$$

Using these bounds, we get the existence of constants C and D, independent of time, such that (6.2) can be replaced by

$$\hbar^{-1} \int_0^T \|\chi_1(\cdot,t)\xi_l(\cdot,t,\hbar)\| \, dt \ \leq \ \hbar^{-1} \, D \, \mathrm{e}^{(2v\tau+3\lambda)T} \, \left(C \, l \, \hbar \, \mathrm{e}^{(6\lambda+2v\tau)T} \right)^{l/2}. \tag{8.1}$$

Thus, if we choose $l = g(T)/\hbar$, then (8.1) is bounded by

$$\hbar^{-1}\, D\, \mathrm{e}^{(2v\tau+3\lambda)T}\, \left(C\, g(T)\, \mathrm{e}^{(6\lambda+2v\tau)T} \right)^{g(T)/(2\hbar)},$$

so that we need

$$g(T)\, \mathrm{e}^{(6\lambda+2v\tau)T} \to 0 \text{ and } g(T)/\hbar \to \infty.$$

These demands are satisfied by the choices

$$g(T) \;=\; \mathrm{e}^{-\kappa T} \qquad \text{and} \qquad T \;=\; T' \ln(1/\hbar), \tag{8.2}$$

provided

$$6\lambda + 2v\tau \;<\; \kappa \;<\; 1/T'. \tag{8.3}$$

Note that the prefactor in (8.1) will be of order $\hbar^{-\nu_1}$, for some finite ν_1. It will thus play no role since it follows from these considerations that there exists $\gamma_1 > 0$, such that

$$\hbar^{-1} \int_0^T \|\chi_1(\cdot,t)\xi_l(\cdot,t,\hbar)\|\, dt \;=\; O(\hbar^{-\nu_1}\, \mathrm{e}^{-\gamma_1/\hbar^{1-\kappa T'}}).$$

By a similar argument, we obtain the estimate corresponding to (6.15) with other time–independent constants D' and C':

$$\hbar^{-1} \int_0^T \|\chi_2(\cdot,t)\xi_l(\cdot,t,\hbar)\|\, dt \;\leq\; \hbar^{-1}\, \mathrm{e}^{-b^2/(12\hbar \mathrm{e}^{2\lambda T})}\, D' \left(C'\, l\, \hbar\, \mathrm{e}^{(8\lambda+2v\tau)T} \right)^{l/2}. \tag{8.4}$$

Inserting our choices (8.2) and constraints (8.3) in (8.4), it is elementary to see that there exists positive ν_2 and γ_2, such that

$$\hbar^{-1} \int_0^T \|\chi_2(\cdot,t)\xi_l(\cdot,t,\hbar)\|\, dt \;=\; O(\hbar^{-\nu_2}\, \mathrm{e}^{-\gamma_2/\hbar^{1-2\lambda T'}}),$$

which proves the Theorem. ■

Proof of Theorem 3.4: Considerations similar to those in the second part of the proof of Theorem 3.3 show that there exists constants C_0, C_1 independent of T such that

$$\begin{aligned}
&\|\chi_2(\cdot,t)\psi(\cdot,t,\hbar)\| \\
&\leq \sum_{k=0}^{l-1} \hbar^{k/2}\, \|c_k(t)\| \left(\sum_{|j|\leq J+3k} \|\chi_2(\cdot,t)\, \phi_j(A(t),B(t),\hbar,a(t),\eta(t),\cdot)\|^2 \right)^{1/2} \\
&\leq \mathrm{e}^{-b^2/(12\hbar \mathrm{e}^{2\lambda T})} \sum_{k=0}^{g(T)/\hbar} \left(\hbar k \mathrm{e}^{(2v\tau+6\lambda)T} C_0 \right)^{k/2} \;\leq\; \mathrm{e}^{-b^2/(12\hbar \mathrm{e}^{2\lambda T})} \sum_{k=0}^{\infty} C_1^k,
\end{aligned}$$

where, by virtue of (8.2) and (8.3), we can take $C_1 < 1$. So, the Theorem holds with exponential decay of order $\mathrm{e}^{-b^2/(12\hbar^{(1-2\lambda\kappa T')})}$. ■

9 Scattering Theory

In this section we show our approximations are valid up to exponentially small corrections in a scattering framework, provided the potential satisfies hypothesis D.

Proof of Theorem 3.5: First note that equations (3.2) together with

$$\mathrm{e}^{-itH_0(\hbar)/\hbar}\,\phi_j(A,B,\hbar,a,\eta,x) \;=\; \mathrm{e}^{it\eta^2/(2\hbar)}\,\phi_j(A+tiB,B,\hbar,a+t\eta,\eta,x)$$

for any $j\in\mathbf{N}^d$ imply that as $t\to\pm\infty$,

$$\mathrm{e}^{itH_0(\hbar)/\hbar}\,\mathrm{e}^{iS(t)/\hbar}\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)\;\to\;\mathrm{e}^{iS_\pm/\hbar}\,\phi_j(A_\pm,B_\pm,\hbar,a_\pm,\eta_\pm,x)$$

with $S_-=0$, for any $j\in\mathbf{N}^d$. Moreover, using (3.2) and the property

$$\min(|v|,1)\,\langle t\rangle\;\le\;\langle tv\rangle\;\le\;\max(|v|,1)\,\langle t\rangle,$$

for any $v\in I\!R^d$ and any $t\in I\!R$, with $\langle t\rangle=\sqrt{1+t^2}$, we get the existence of $\tilde c_0>0$ and $\tilde c_1>0$ depending on the asymptotic data $(a_\pm,\eta_\pm)$, such that

$$\left|\frac{D^mV(a(t))}{m!}\right|\;\le\;\frac{\tilde c_0\,\tilde c_1^{|m|}}{\langle t\rangle^{\beta+|m|}} \tag{9.1}$$

for large times. This estimate together with (3.3) and Lemma 5.1 yields the following estimate on the operator $K_k(t)\,P_{|j|\le n}$ defined in (4.6):

$$\begin{aligned}\|K_k(t)\,P_{|j|\le n}\| &= \left\|\sum_{|m|=k}\frac{D^mV(a(t))}{m!}\,X(t)^m\,P_{|j|\le n}\right\|\\ &\le \binom{d-1+k}{d-1}\sqrt{\frac{(n+k)!}{n!}}\;\frac{\tilde c_0\,\tilde c_2^k}{\langle t\rangle^\beta}\,,\end{aligned} \tag{9.2}$$

where $\tilde c_2$ depends on the asymptotic data $(a_\pm,\eta_\pm,A_\pm,B_\pm)$ and the binomial coefficient gives the number of multi-indices of order k. At the possible cost of an increase in the constants, we may assume this estimate is valid for all $t\in I\!R$.

This estimate shows in particular that $K_k(t)\,P_{|j|\le n}$ is integrable in time. From this, it is easy to check inductively that the solutions $c_n(t)$ to the equations (4.11) have limits as $|t|\to\infty$.

The asymptotic values of the coefficients $c_n(t)$ at infinity allow us to define the asymptotic states $\Phi_\pm(A_\pm,B_\pm,\hbar,a_\pm,\eta_\pm,x)$ by (3.6) with initial conditions at $-\infty$ characterized by arbitrary normalized coefficients that satisfy

$$\begin{aligned} c_{0,j}(-\infty) &= 0, \quad \text{for } |j|>J, \quad \text{and}\\ c_{n,j} &= 0, \quad \text{for } n=1,2,\cdots,\ \text{and all } j\in\mathbf{N}^d.\end{aligned} \tag{9.3}$$

Thus, our approximate solution

$$\psi(x,t,\hbar)\;=\;e^{iS(t)/\hbar}\sum_{|j|\le J+3g/\hbar-3} c_j(t,\hbar)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)$$

has the asymptotic property as $t \to \pm\infty$,

$$\mathrm{e}^{itH_0(\hbar)/\hbar}\,\psi(x,t,\hbar)\;\to\;\Phi_\pm(A_\pm,B_\pm,\hbar,a_\pm,\eta_\pm,x). \tag{9.4}$$

We prove below that

$$\begin{aligned}
&\|\psi(x,t,\hbar)\;-\;\lim_{s\to\infty}\,\mathrm{e}^{i(t-s)H(\hbar)/\hbar}\,\mathrm{e}^{isH_0(\hbar)/\hbar}\,\Phi_-(A_-,B_-,\hbar,a_-,\eta_-,x)\|\\
=\;&\|\psi(x,t,\hbar)\;-\;\mathrm{e}^{itH(\hbar)/\hbar}\,\Omega^+(\hbar)\,\Phi_-(A_-,B_-,\hbar,a_-,\eta_-,x)\|\\
=\;&O(\mathrm{e}^{-\gamma/\hbar}),
\end{aligned}$$

uniformly for $t\in I\!\!R$. Thus, making use of (9.4), we have

$$\begin{aligned}
&\lim_{t\to+\infty}\,\|\mathrm{e}^{itH_0(\hbar)/\hbar}\,\psi(x,t,\hbar)\;-\;\mathrm{e}^{itH_0(\hbar)/\hbar}\,\mathrm{e}^{itH(\hbar)/\hbar}\,\Omega^+(\hbar)\,\Phi_-(A_-,B_-,\hbar,a_-,\eta_-,x)\|\\
=\;&\|\Phi_+(A_+,B_+,\hbar,a_+,\eta_+,x)\;-\;\Omega^-(\hbar)^*\,\Omega^+(\hbar)\,\Phi_-(A_-,B_-,\hbar,a_-,\eta_-,x)\|\\
=\;&\|\Phi_+(A_+,B_+,\hbar,a_+,\eta_+,x)\;-\;S(\hbar)\,\Phi_-(A_-,B_-,\hbar,a_-,\eta_-,x)\|\\
=\;&O(\mathrm{e}^{-\gamma/\hbar}).
\end{aligned}$$

Hence, we need only show that the estimate on $\xi_l(x,t,\hbar)$ corresponding to our approximation yields an exponentially small correction term after choosing $l=g/\hbar$ for sufficiently small g, uniformly for $t\in I\!\!R$.

We mimic Section 5 to get estimates on the coefficients

$$c_k(t)\;=\;\sum_{p=1}^{k}\,c_k^{[p]}(t) \tag{9.5}$$

starting with

$$c_{0,j}(t)=c_{0,j}(-\infty),\qquad c_{0,j}(-\infty)=0\quad\text{if }|j|>J,\qquad\text{and}\qquad\|c_0(-\infty)\|\;=\;1.$$

We note that the number of components of the vectors $c_k^{[p]}(t)$ is the same as in (5.8) and that the combinatorics associated with the n and p dependence of the estimates is identical to that performed in Section 5.

Hence, with $D_3=\begin{pmatrix}d+2\\ d-1\end{pmatrix}$, at first order we have

$$\|c_1(t)\|\;=\;\|c_1^{[1]}(t)\|\;\le\;D_3\,\sqrt{\frac{(J+3)!}{J!}}\;\tilde{c}_0\,\tilde{c}_2^3\,\int_{-\infty}^{t}\langle s\rangle^{-\beta}\,ds.$$

At second order, we obtain $c_2(t)=c_2^{[1]}(t)+c_2^{[2]}(t)$, where

$$\|c_2^{[1]}(t)\|\;\le\;D_3^2\,\sqrt{\frac{(J+4)!}{J!}}\;\tilde{c}_0\,\tilde{c}_2^4\,\int_{-\infty}^{t}\langle s\rangle^{-\beta}\,ds\qquad\text{and}$$

$$\|c_2^{[2]}(t)\|\;\le\;D_3^2\,\sqrt{\frac{(J+6)!}{J!}}\;\tilde{c}_0^2\,\tilde{c}_2^6\,\int_{-\infty}^{t}ds_1\,\langle s_1\rangle^{-\beta}\int_{-\infty}^{s_1}ds_2\,\langle s_2\rangle^{-\beta}.$$

At third order, we obtain $c_3(t) = c_3^{[1]}(t) + c_3^{[2]}(t) + c_3^{[3]}(t)$, where

$$\begin{aligned}
\|c_3^{[1]}(t)\| &\leq D_3^3 \sqrt{\frac{(J+5)!}{J!}}\ \tilde{c}_0\, \tilde{c}_2^5 \int_{-\infty}^t \langle s\rangle^{-\beta}\, ds, \\
\|c_3^{[2]}(t)\| &\leq 2\, D_3^3 \sqrt{\frac{(J+7)!}{J!}}\ \tilde{c}_0^2\, \tilde{c}_2^7 \int_{-\infty}^t ds_1\, \langle s_1\rangle^{-\beta} \int_{-\infty}^{s_1} ds_2\, \langle s_2\rangle^{-\beta}, \qquad \text{and} \\
\|c_3^{[3]}(t)\| &\leq D_3^3 \sqrt{\frac{(J+9)!}{J!}}\ \tilde{c}_0^3\, \tilde{c}_2^9 \int_{-\infty}^t ds_1\, \langle s_1\rangle^{-\beta} \int_{-\infty}^{s_1} ds_2\, \langle s_2\rangle^{-\beta} \int_{-\infty}^{s_2} ds_3\, \langle s_3\rangle^{-\beta}.
\end{aligned}$$

Using the identity

$$\int_{-\infty}^t ds_1\, \langle s_1\rangle^{-\beta} \int_{-\infty}^{s_1} ds_2\, \langle s_2\rangle^{-\beta} \cdots \int_{-\infty}^{s_{n-1}} ds_n\, \langle s_n\rangle^{-\beta} \;=\; \frac{1}{n!}\, \left(\int_{-\infty}^t \langle s\rangle^{-\beta}\, ds \right)^n,$$

we get estimates identical to (5.11), (5.14), (5.15), (5.20), (5.21), (5.22).

It is easy to check that the induction can be carried out exactly as in Section 5 to give an analog of Corollary 5.3 that states

Lemma 9.1 *Assume the decay hypothesis D. The expansion coefficients (9.5) satisfying (9.3) obey the following estimates:*

$$\begin{aligned}
c_{k,j}(t) &= 0, \qquad \text{whenever} \quad |j| > J + 3k, \\
\|c_k^{[p]}(t)\| &\leq \binom{k-1}{p-1}\ D_3^k \sqrt{\frac{(J+3k)!}{J!}}\ \tilde{c}_0^p\ \tilde{c}_2^{k+2p}\ \frac{\left(\int_{-\infty}^t ds\, \langle s\rangle^{-\beta}\right)^p}{k!}
\end{aligned}$$

for $p \leq k$, and

$$\|c_k(t)\| \leq \sqrt{\frac{(J+3k)!}{J!}}\ \frac{\tilde{c}_2^k\, D_3^k}{k!} \left(1 + \tilde{c}_0 \tilde{c}_2^2 \int_{-\infty}^t ds\, \langle s\rangle^{-\beta}\right)^{k-1} \tilde{c}_0\ \tilde{c}_2^2 \int_{-\infty}^t ds\, \langle s\rangle^{-\beta}.$$

Our next task is to estimate the norm of $\xi_l(x,t)$. We again consider separately the errors near the classical orbit and those far from the orbit. Let $b(t)$ be a real valued function that satisfies

$$\frac{\langle a(t)\rangle}{4} \;\leq\; b(t) \;\leq\; \frac{\langle a(t)\rangle}{2}, \tag{9.6}$$

for all $t \in I\!R$. We define $\chi_1(x,t)$ to be the characteristic function of $\{x : |x - a(t)| \leq b(t)\}$ and $\chi_2(x,t) = 1 - \chi_1(x,t)$. Then, for some constants $\tilde{c}_3$ and $\tilde{c}_4$ and any $t \in I\!R$, we have

$$\begin{aligned}
\left| \frac{D^m V(\zeta_m(x, a(t)))}{m!}\, \chi_1(x,t)) \right| &\leq \frac{v_0\ v_1^{|m|}}{\langle \zeta_m(x, a(t)))\rangle^{\beta+|m|}}\ \chi_1(x,t) \\
&\leq \frac{\tilde{c}_3\ \tilde{c}_4^{|m|}}{\langle t\rangle^{\beta+|m|}},
\end{aligned}$$

since for large times on the support of χ_1,

$$|\zeta_m(x, a(t)))| \;\geq\; |a(t)|/4.$$

Therefore, for some constants $\tilde{c}_5$ and $\tilde{c}_6$,

$$\left\| \chi_1(x,t)\, \frac{D^m V(\zeta_m(x,a(t)))}{m!}\, X(t)^m\, P_{|j|\le n} \right\| \;\le\; \sqrt{\frac{(n+|m|)!}{n!}}\; \frac{\tilde{c}_5\, \tilde{c}_6^{|m|}}{\langle t\rangle^{\beta}},$$

for any $t \in I\!\!R$. We now mimic the manipulations performed in Section 6 to get

$$\begin{aligned}
&\|\, \chi_1(x,t)\, \xi_l(x,t,\hbar)\, \| \qquad (9.7)\\
\le\;& \Bigg\| \sum_{k=0}^{l-1} \sum_{|m|=l+2-k} \hbar^{k/2}\, \chi_1(x,t)\, \frac{(D^m V)(\zeta_m(x,a(t))}{m!}\, \hbar^{|m|/2}\, (x-a(t))^m\, \hbar^{-|m|/2} \\
&\qquad \times\; P_{|j|\le J+3k} \sum_{|j|\le J+3k} c_{k,j}(t)\, \phi_j(A(t),B(t),\hbar,a(t),\eta(t),x) \Bigg\| \\
\le\;& \sum_{k=0}^{l-1} \hbar^{(l+2)/2} \binom{d-1+l+2-k}{d-1}\, \|c_k(t)\| \\
&\qquad \times \max_{\{m\,:\ |m|=l+2-k\}} \left\| \chi_1(x,t)\, \frac{D^m V(\zeta_m(x,a(t)))}{m!}\, X(t)^m\, P_{|j|\le J+3k} \right\| \\
\le\;& \sum_{k=0}^{l-1} \hbar^{(l+2)/2} \binom{d-1+l+2-k}{d-1} \sqrt{\frac{(J+2k+l+2)!}{J!}}\; \frac{\tilde{c}_5\, \tilde{c}_6^{l+2-k}}{\langle t\rangle^{\beta}} \\
&\qquad \times\; \frac{\tilde{c}_2^k\, D_3^k}{k!} \left(1+\tilde{c}_0\tilde{c}_2^2 \int_{-\infty}^{t} ds\, \langle s\rangle^{-\beta}\right)^{k-1} \tilde{c}_0\, \tilde{c}_2^2 \int_{-\infty}^{t} ds\, \langle s\rangle^{-\beta}.
\end{aligned}$$

Making use of (5.30), the definition of D_3, and introducing another constant

$$\tilde{c}_7 \;=\; \left(1 \,+\, \tilde{c}_0\, \tilde{c}_2^2\, I\right) \tilde{c}_2/\tilde{c}_6, \qquad \text{where} \qquad I \;=\; \int_{-\infty}^{\infty} \langle s\rangle^{-\beta}\, ds,$$

(9.7) is bounded by

$$\begin{aligned}
&\frac{\tilde{c}_5\, \tilde{c}_0\, (\tilde{c}_6\, \tilde{c}_2)^2\, I}{\sqrt{J!}\, \langle t\rangle^{\beta}}\, \hbar^{(l+2)/2}\, (\tilde{c}_6\, D_3)^l \sum_{k=0}^{l-1} \tilde{c}_7^k\, \frac{\sqrt{(J+2k+l+2)!}}{k!} \\
\le\;& \frac{\tilde{c}_5\, \tilde{c}_0\, (\tilde{c}_6\, \tilde{c}_2)^2\, I}{\sqrt{J!}\, \langle t\rangle^{\beta}}\, \hbar^{(l+2)/2}\, (\tilde{c}_6\, D_3)^l \sum_{k=0}^{l-1} \tilde{c}_7^k\, \frac{\sqrt{(J+3l)!}}{(l-1)!} \\
\le\;& \frac{\tilde{c}_5\, \tilde{c}_0\, (\tilde{c}_6\, \tilde{c}_2)^2\, I}{(\tilde{c}_7-1)\, \sqrt{J!}\, \langle t\rangle^{\beta}}\, \hbar^{(l+2)/2}\, (\tilde{c}_6\, D_3 \tilde{c}_7)^l\, \frac{\sqrt{(J+3l)!}}{(l-1)!} \\
=\;& \frac{\tilde{c}_5\, \tilde{c}_0\, (\tilde{c}_6\, \tilde{c}_2)^2\, I}{(\tilde{c}_7-1)\sqrt{J!}\, \langle t\rangle^{\beta}}\, \hbar^{(l+2)/2} \left(D_3 \left(1+\tilde{c}_0\tilde{c}_2^2 I\right) \tilde{c}_2\right)^l \frac{\sqrt{(J+3l)!}}{(l-1)!}. \qquad (9.8)
\end{aligned}$$

This estimate is integrable for $t \in I\!\!R$ and yields a bound that implies exponential decay in $\hbar$ by the optimal truncation technique.

We now come to the estimate of $\|\chi_2(x,t)\xi_l(x,t)\|$, which is a little bit more elaborate. The difficulty stems from a lack of sufficient information on the position of $\zeta_m(x,a(t))$. So, instead of the usual Taylor series error formula, we use the definition

$$W_{a(t)}^{(q)}(x) = V(x) - \sum_{|m|\leq q} \frac{D^m V(a(t))}{m!} (x-a(t))^m.$$

We ultimately use $q = l+1-k$, where $k = 0, 1, \cdots, l-1$. Our proof requires the space dimension to satisfy $d \geq 3$ in order to obtain integrability in t.

Consider the following integral

$$\begin{aligned} N^2 &= \int_{I\!R^d} \chi_2(x,t)^2 \, |\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)|^2 \, V(x)^2 \, dx \\ &= \int_{|z|\geq b(t)} |\phi_j(A(t),B(t),\hbar,0,0,z)|^2 \, V(z+a(t))^2 \, dz. \end{aligned}$$

We use the formula

$$|\phi_j(A(t),B(t),\hbar,0,0,z)| = \frac{\mathrm{e}^{-(|A|^{-1}(t)z)^2/2\hbar} \, |\mathcal{H}_j(A;\, |A(t)|^{-1}\hbar^{1/2} z)|}{\sqrt{j!\, 2^{|j|}\, \pi^{d/2}\, |\det A(t)|\, \hbar^{d/2}}},$$

the asymptotic behavior (3.3), and the following estimate, which is valid on the support of χ_2,

$$(|A(t)|^{-1}z)^2 \;\geq\; \frac{z^2}{\|A(t)\|^2} \;\geq\; \frac{b^2(t)}{\|A(t)\|^2} \;\geq\; \frac{\langle a(t)\rangle^2}{16\,\|A(t)\|^2}$$

to obtain the bound

$$N^2 \;\leq\; \mathrm{e}^{-\tilde{b}/\hbar} \int_{|z|\geq b(t)} \frac{\mathrm{e}^{-(|A(t)|^{-1}z)^2/2\hbar} \, |\mathcal{H}_j(A;\, |A(t)|^{-1}\hbar^{1/2} z)|^2}{j!\, 2^{|j|}\, \pi^{d/2}\, |\det A(t)|\, \hbar^{d/2}} \, V(z+a(t))^2 \, dz,$$

for some finite, positive $\tilde{b}$. Note that this estimate has a uniform exponentially decreasing prefactor.

As in Section 6, we use spherical coordinates and the decomposition (6.20)

$$\Omega_j(y) \;=\; \sum_{\{q,n,m:\, 2n+q=|j|\}} d_{j,q,n,m}\, \psi_{q,n,m}(r,\omega),$$

where $\displaystyle\sum_{\{q,n,m:\, 2n+q=|j|\}} |d_{j,q,n,m}|^2 \;=\; 1$ and $\Omega_j(y) \;=\; \sqrt{\dfrac{1}{2^{|j|}\, j!\, \pi^{d/2}}}\, \mathcal{H}_j(A;\, y)\, \mathrm{e}^{-y^2/2}$. This leads to the estimate

$$N^2 \;\leq\; \mathrm{e}^{-\tilde{b}/\hbar} \sum_{\{q,n,m:\, 2n+q=|j|\}} \int_{|z|\geq b(t)} \frac{\mathrm{e}^{+(|A(t)|^{-1}z)^2/2\hbar} \, |\,\psi_{q,n,m}(r_z,\omega_z)|^2}{|\det A(t)|\, \hbar^{d/2}} \, V(z+a(t))^2 \, dz,$$

where the spherical coordinates (r_z, ω_z) describe the vector $\hbar^{1/2}\, |A(t)|^{-1}\, z$.

We choose $p > 2$, such that $d/\beta < p < d$, and define $s > 2$ by $1/s + 1/p = 1/2$. Applying Hölder's inequality, we get the bound

$$N^2 \;\leq\; \frac{\mathrm{e}^{-\tilde{b}/\hbar}}{|\det A(t)|\, \hbar^{d/2}} \sum_{\{q,n,m:\, 2n+q=|j|\}} \|V\|_p^2 \left(\int_{|z|\geq b(t)} \mathrm{e}^{+(|A(t)|^{-1}z)^2 s/4\hbar}\, |\psi_{q,n,m}(r_z,\omega_z)|^s dz \right)^{2/s}.$$

We need to bound the integral in this expression. We change variables to $y = |A(t)|^{-1} z/\hbar^{1/2}$ and use the estimate $|\,|A(t)|y\,| \le b(t)/\sqrt{\hbar}$, which is valid when $|y| \le b(t)/(\|A(t)\|\sqrt{\hbar})$. This yields

$$\begin{aligned}
&\int_{|z|\ge b(t)} \mathrm{e}^{+(|A(t)|^{-1}z)^2 s/4\hbar}\, |\psi_{q,n,m}(r_z,\omega_z)|^s\, dz \\
\le\ &\int_{|y|\ge \frac{b(t)}{\|A(t)\|\sqrt{\hbar}}} \mathrm{e}^{+y^2 s/4}\, |\psi_{q,n,m}(r,\omega)|^s\, |\det A(t)|\, \hbar^{d/2}\, dy,
\end{aligned} \tag{9.9}$$

where the spherical coordinates (r,ω) now describe the vector y. Note that we have used $\det(|A|) = |\det(A)|$, which follows from $A = U_A\,|A|$, where U_A is unitary.

Since $b(t)/\|A(t)\|$ has a strictly positive infimum $\bar{b}$, and we ultimately choose $l \simeq g/\sqrt{\hbar}$, with g arbitrarily small, we can assume the integration in (9.9) is within the classically forbidden region where Lemma 4.2 applies, for all indices $\{q,n,m:\ 2n+q = |j|\}$ of interest.

Hence, manipulations similar to those performed in Section 6, show that (9.9) is bounded above by

$$\begin{aligned}
&\frac{|\det A(t)|\,\hbar^{d/2}\,2^{s/2}}{\Gamma(q+n+d/2)^{s/2}\,n!^{s/2}} \int_{S^{d-1}} d\omega\,|Y_{q,m}|^s \int_{\bar{b}/\sqrt{\hbar}}^{\infty} dr\, r^{d-1+sq+2sn}\, \mathrm{e}^{-sr^2/4} \\
\le\ &\frac{|\det A(t)|\,\hbar^{d/2}\,(2/s)^{d+s|j|}\,2^{s/2}}{\Gamma(q+n+d/2)^{s/2}\,n!^{s/2}} \int_{S^{d-1}} d\omega\,|Y_{q,m}|^s \int_0^{\infty} dz\, z^{d-1+s|j|}\, \mathrm{e}^{-z^2} \\
\le\ &\frac{|\det A(t)|\,\hbar^{d/2}\,(2/s)^{d+s|j|}\,2^{s/2}}{\Gamma(q+n+d/2)^{s/2}\,n!^{s/2}} \int_{S^{d-1}} d\omega\,|Y_{q,m}|^s\, \Gamma\left(\frac{d+s|j|}{2}\right)/2.
\end{aligned}$$

This implies the estimate

$$\begin{aligned}
N^2 \ \le\ &\frac{\mathrm{e}^{-\tilde{b}/\hbar}\,\|V\|_p^2\,(2/s)^{2(d/s+|j|)}\,\Gamma\left((d+s|j|)/2\right)^{2/s}}{2^{2/s-1}\,|\det A(t)|^{1-2/s}\,\hbar^{d/2-d/s}} \\
&\times\ \left(\sum_{\{q,n,m:\,2n+q=|j|\}} \frac{\int_{S^{d-1}} d\omega\,|Y_{q,m}|^s}{\Gamma(q+n+d/2)^{s/2}\,n!^{s/2}}\right)^{2/s}.
\end{aligned}$$

We bound the integral in this expression by using the following crude lemma. Its proof is at the end of this section.

Lemma 9.2 *For some constants M_0 and M_1, we have*

$$|\,Y_{q,m}(\omega)\,| \ \le\ M_0\ M_1^q. \tag{9.10}$$

We use this and the inequalities $q \le |j|$ and $\binom{|j|}{n} \le 2^{|j|}$ to estimate

$$\left(\sum_{\{q,n,m:\,2n+q=|j|\}} \frac{\int_{S^{d-1}} d\omega\,|Y_{q,m}|^s}{\Gamma(q+n+d/2)^{s/2}\,n!^{s/2}}\right)^{2/s}$$

$$\leq \quad \frac{M_0^2\,|S^{d-1}|^{2/s}\,(2dM_1^2)^{|j|}\,m_{|j|}^{2/s}}{\pi^{d/2}} \left(\sum_{n=0}^{|j|/2} \frac{1}{\Gamma(|j|-n+d/2)^{s/2}\,n!^{s/2}}\right)^{2/s}$$

$$\leq \quad \frac{M_0^2\,|S^{d-1}|^{2/s}\,(2dM_1^2)^{|j|}\,m_{|j|}^{2/s}}{\pi^{d/2}\,C''\,|j|!} \left(\sum_{n=0}^{|j|/2} \binom{|j|}{n}^{s/2}\right)^{2/s}$$

$$\leq \quad \frac{|j|^{2/s}\,M_0^2\,|S^{d-1}|^{2/s}\,(4dM_1^2)^{|j|}\,m_{|j|}^{2/s}}{\pi^{d/2}\,C''\,|j|!}.$$

Hence, for some constants N_0 and N_1, that depend on d and s only,

$$N \;\leq\; \mathrm{e}^{-\tilde{b}/2\hbar}\,\frac{\|V\|_p\,N_0\,N_1^{|j|}}{|\det A(t)|^{1/p}\,\hbar^{d/p}}.$$

By our choice of p,

$$\frac{1}{|\det A(t)|^{1/p}} \;\simeq\; 1/\langle t\rangle^{d/p}$$

is integrable.

For $k \leq l \simeq g/\hbar$, with sufficiently small g, this last estimate allows us to bound the corresponding term in $\|\xi_l(x,t)\chi_2(x,t)\|$ as follows (where the N_i, $i=0,1,2,3\ldots$ are constants):

$$\begin{aligned}
& \sum_{k=0}^{l-1} \hbar^{k/2} \left\| \sum_{|j|\leq J+3k} c_{k,j}(t)\,\chi_2(x,t)\,V(x)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x) \right\| \\
\leq\;& \sum_{k=0}^{l-1} \hbar^{k/2}\,\|c_k(t)\| \left(\sum_{|j|\leq J+3k} \|V(x)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)\| \right)^{1/2} \\
\leq\;& \sum_{k=0}^{l-1} \hbar^{k/2} \sqrt{\frac{(J+3k)!}{J!}}\;\frac{N_3^k}{k!}\;\mathrm{e}^{-\tilde{b}/2\hbar}\;\frac{\|V\|_p\,N_0}{|\det A(t)|^{1/p}\,\hbar^{d/p}} \left(\sum_{|j|\leq J+3k} N_1^{2|j|} \right)^{1/2} && (9.11) \\
\leq\;& \frac{\mathrm{e}^{-\tilde{b}/2\hbar}\,N_4}{|\det A(t)|^{1/p}\,\hbar^{d/p}} \sum_{k=0}^{l-1} k^{k/2}\,\hbar^{k/2}\,N_5^k \\
\leq\;& \frac{\mathrm{e}^{-\tilde{b}/2\hbar}\,N_6}{|\det A(t)|^{1/p}\,\hbar^{d/p}}. && (9.12)
\end{aligned}$$

It remains for us to control integrals of the form

$$\begin{aligned}
F^2(p) \;&=\; \int_{I\!R^d} \chi_2^2(x,t)|\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)|^2 |D^pV(a(t))(x-a(t))^p|^2/(p!)^2\,dx \\
&\leq\; \frac{\tilde{c}_0^2\,\tilde{c}_1^{2|p|}}{\langle t\rangle^{2(\beta+|p|)}} \int_{|x-a(t)|\geq b(t)} (x-a(t))^{2|p|}\,|\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)|^2\,dx \\
&\leq\; \frac{\tilde{c}_0^2\,\tilde{c}_2^{2|p|}\,\mathrm{e}^{-\tilde{b}/(2\hbar)}\,\hbar^{|p|}}{\langle t\rangle^{2\beta}} \int_{|y|\geq\tilde{b}/\sqrt{\hbar}} y^{2|p|}|\,\mathcal{H}_j(A;y)|^2\,\mathrm{e}^{y^2/2}/(2^{|j|}\,j!\,\pi^{d/2})\,dy,
\end{aligned}$$

where we used the same type of estimates as above. We bound the last integral in this expression by using spherical coordinates and noting that the integration region lies within the classically forbidden region, if g is sufficiently small. The integral is thus bounded by

$$\sum_{\{q,n,m\,:\,2n+q=|j|\}} \frac{2^{2n+q+|p|+d/2-1}}{n!\,\Gamma(q+n+d/2)}\,\Gamma(2n+q+|p|+d/2) \;\leq\; f_0\, f_1^{|p|}\,(|j|+|p|)!/|j|!.$$

So, for some other constants we have

$$F(p)^2 \;\leq\; \frac{f_2\, f_3^{|j|}\, f_4^{|p|}\,\hbar^{|p|}\,\mathrm{e}^{-\tilde{b}/(2\hbar)}\,(|j|+|p|)!}{\langle t\rangle^{2\beta}\,|j|!}.$$

The corresponding sum in $\|\chi_2\xi_l\|$ is bounded by

$$\begin{aligned}
&\left\| \sum_{k=0}^{l-1} h^{k/2} \sum_{|j|\leq J+3k} c_{k,j}(t) \right.\\
&\qquad \left. \times \sum_{|p|\leq l+1-k} \chi_2(x,t)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x)\,\frac{D^pV(a(t))\,(x-a(t))^p}{p!}\right\|\\
&\leq\; \sum_{k=0}^{l-1} h^{k/2} \sum_{|p|\leq l+1-k} \|c_k(t)\| \left(\sum_{|j|\leq J+3k} F^2(p)\right)^{1/2}\\
&\leq\; \sum_{k=0}^{l-1} h^{k/2} f_5^k\, \frac{\sqrt{(J+3k)!}}{\sqrt{J!}\,k!} \sum_{|p|\leq l+1-k}\left(\sum_{|j|\leq J+3k} \frac{f_2 f_3^{J+3k} f_4^{|p|}\hbar^{|p|}\mathrm{e}^{-\tilde{b}/(2\hbar)}(J+3k+|p|)!}{\langle t\rangle^{2\beta}\,(J+3k)!}\right)^{1/2}\\
&\leq\; \frac{\mathrm{e}^{-\tilde{b}/(4\hbar)}}{\langle t\rangle^{\beta}}\,\frac{f_2^{1/2}\,\mathrm{e}^{\bar{\beta}J}}{\sqrt{J!}} \sum_{k=0}^{l-1} \frac{h^{k/2}\, f_6^k}{k!} \sum_{|p|\leq l+1-k} \hbar^{|p|/2}\, f_7^{|p|}\,\sqrt{(J+3k+|p|)!},
\end{aligned} \tag{9.13}$$

where $\bar{\beta}$ is independent of J. The last sum in this expression is bounded by

$$\sum_{r=0}^{l+1-k} (f_8\hbar^{1/2})^r\,\sqrt{(J+3k+r)!} \;=\; \sum_{s=3k}^{l+1+2k} (f_8\,\hbar^{1/2})^s\,\sqrt{(J+s)!}\,(f_8\,\hbar^{1/2})^{-3k}. \tag{9.14}$$

Since $s\leq l+1+2k\leq 3l+1\simeq g/\hbar$ and g is small, we have

$$(f_8\,\hbar^{1/2})^s\,\sqrt{(J+s)!} \;\leq\; (f_9\,\hbar^{1/2}\,s^{1/2})^s \;\leq\; \alpha(g)^s,$$

where $\alpha(g)=f_{10}\sqrt{g}$ is smaller than one. Furthermore, the sum (9.14) is bounded by

$$\frac{\alpha(g)^{3k}}{1-\alpha(g)}\,(f_8\,\hbar^{1/2})^{-3k}.$$

From this we deduce that (9.13) is dominated by a constant times

$$\begin{aligned}
\frac{\mathrm{e}^{-\tilde{b}/(4\hbar)}}{\langle t\rangle^{\beta}} \sum_{k=0}^{l-1} \frac{h^{k/2}\, f_6^k}{k!}\, 2\,\alpha(g)^{3k}\,(f_8\,\hbar^{1/2})^{-3k} \;&=\; 2\,\frac{\mathrm{e}^{-\tilde{b}/(4\hbar)}}{\langle t\rangle^{\beta}} \sum_{k=0}^{l-1} \frac{\tilde{\alpha}(g)^k}{\hbar^k\,k!}\\
&\leq\; 2\,\frac{\mathrm{e}^{-\tilde{b}/(4\hbar)}}{\langle t\rangle^{\beta}}\,\mathrm{e}^{\tilde{\alpha}(g)/\hbar}\\
&\leq\; \frac{\mathrm{e}^{-\tilde{b}/(8\hbar)}}{\langle t\rangle^{\beta}},
\end{aligned} \tag{9.15}$$

provided g is small enough, since $\tilde{\alpha}(g) \simeq g^{3/2}$ as $g \to 0$, which is exponentially small and integrable in time.

Finally, gathering estimates (9.8), (9.12) and (9.15), we get the existence of positive γ, H, G, and C, such that $g < G$, $l(\hbar) = g/\hbar$, and $\hbar < H$ imply

$$\int_{-\infty}^{\infty} dt\, \|\xi_l(x,t)\|/\hbar \ \leq\ C\,\mathrm{e}^{-\gamma/\hbar}.$$

Proof of Lemma 9.2: Let $f \in \mathcal{S}$ be the function that is given in spherical coordinates by

$$f(x) \ =\ \sqrt{\frac{2}{\Gamma(q+\frac{d}{2})}}\ r^q\ e^{-r^2/2}\ Y_{q,m}(\omega).$$

For integers $q > 0$, the maximum absolute value of this function is

$$\sqrt{\frac{2}{\Gamma(q+\frac{d}{2})}}\ q^{q/2}\ e^{-q/2}\ \max_{\omega}\ |\,Y_{q,m}(\omega)\,|. \tag{9.16}$$

The function f is a normalized eigenfunction of $-\Delta + x^2$ with eigenvalue $E = 2q + d$. Its norm in the Sobolev space $\mathcal{H}_s$ for $s > 0$ satisfies

$$\|f\|_{\mathcal{H}_s}\ \leq\ C_1(s)\ \Big(\|f\| + \|(-\Delta)^{s/2} f\|\Big)\ \leq\ C_1(s)\ \Big(1\ +\ (2q+d)^{s/2}\Big)\,, \tag{9.17}$$

for some $C_1(s)$.

If $s > d/2$, then $(1+|k|^2)^{-s/2}$ is in $L^2(I\!\!R^d)$. So, by Hölder's inequality,

$$|\,f(x)\,|\ \leq\ (2\pi)^{-d/2}\ \left\|\,\widehat{f}(k)\,(1+|k|^2)^{s/2}\,\right\|\ \left\|\,(1+|k|^2)^{-s/2}\,\right\|\ =\ C_2(s)\ \|f\|_{\mathcal{H}_s}.$$

This and (9.17) imply that (9.16) is bounded by $C_3(s)\ \Big(1\ +\ (2q+d)^{s/2}\Big)$. Thus,

$$\max_{\omega}\ |\,Y_{q,m}(\omega)\,|\ \leq\ C_3(s)\ \sqrt{\frac{\Gamma(q+\frac{d}{2})}{2}}\ \ \Big(1\ +\ (2q+d)^{s/2}\Big)\ q^{-q/2}\ e^{q/2}.$$

The lemma follows from this by an application of Stirling's formula. ∎

10 More General Coherent States

In this section we extend all the previous theorems of the paper to allow initial conditions that are certain infinite linear combinations of the ϕ_j.

Proof of Theorem 3.6: The strategy is quite simple. Let $\varphi \in \mathcal{C}$ have expansion $\varphi = c_j\,\phi_j(I\!\!I, I\!\!I,\,\hbar,\,0,\,0,\,x)$, and let

$$\psi_0(x,0,\hbar)\ =\ (\Lambda_h(a,\eta)\varphi)(x)$$

be our initial condition. By construction,

$$\psi_0(x,0,\hbar) \;=\; \sum_{j\in\mathbf{N}^d} c_j\,\phi_j(I\!I, I\!I,\,\hbar,\,a,\,\eta,\,x).$$

For $J>0$, we define

$$\psi_J(x,0,\hbar) = \sum_{|j|\le J} c_j\,\phi_j(I\!I, I\!I,\,\hbar,\,a,\,\eta,\,x),$$

and denote the approximation that arises from this initial condition by

$$\psi_{\tilde{J}(J,\hbar)}(x,t,\hbar) \;=\; \sum_{|j|\le\tilde{J}(J,\hbar)} c_j(t,\hbar)\,\phi_j(A(t),B(t),\hbar,a(t),\eta(t),x).$$

We then have

$$\begin{aligned}
&\mathrm{e}^{-itH(\hbar)/\hbar}\,\psi_0(0,\hbar)\\
=\;& \mathrm{e}^{-itH(\hbar)/\hbar}\,(\psi_0(0,\hbar)-\psi_J(0,\hbar))\;+\;\mathrm{e}^{-itH(\hbar)/\hbar}\,\psi_J(0,\hbar) \qquad (10.1)\\
=\;& \psi_{\tilde{J}(J,\hbar)}(t,\hbar)+O(\|\mathrm{e}^{-itH(\hbar)/\hbar}\psi_J(0,\hbar)-\psi_{\tilde{J}(J,\hbar)}(t,\hbar)\|)+O(\|\psi_0(0,\hbar)-\psi_J(0,\hbar))\|).
\end{aligned}$$

Thus, to make the error terms exponentially small in $\hbar$ we need to consider values of the cutoff J that grow to infinity with $\hbar$ in a suitable way, and we also need to control our approximation as a function of J.

In the proofs of all previous theorems, the dependence of the approximation on l governs the estimates on the error terms. The $\hbar$ dependence comes through the different choices of $l\simeq g/\hbar$ or $l\simeq g(T)/\hbar$, with $T\simeq\ln(1/\hbar)$. The set $\mathcal{C}$ is chosen to give an exponentially small contribution as $l\to\infty$ in the last term of (10.1) with the choice

$$J=\nu\,l, \qquad (10.2)$$

for some $\nu>0$. We need only show that the basic estimates in the proofs above are unaltered by the replacement of J by $\nu\,g/\hbar$, for g small enough.

We can do this because we have been careful to make the J dependence explicit in all the key estimates, such as Corollary 5.3.

In the contribution to the error term associated with χ_1 given by (6.8) we adapt the last step by using the estimate

$$\frac{(J(l)+3l)!}{J(l)!}\;\le\;c_0(\nu)\,\frac{((\nu+3)l)^{(\nu+3)l}}{(\nu l)^{\nu l}}\;\le\;c_0(\nu)\,c_1(\nu)^l\,l^{3l}, \qquad (10.3)$$

for some constants $c_0(\nu)$ and $c_1(\nu)$. Hence, the remainder of the argument for Lemma 6.1 is the same, with updated constants. Since the constants are modified in a time independent way, the long time estimates are also unchanged.

Consider now the contribution associated with χ_2 in Lemma 6.3. We first note that (10.2) implies (with a slight abuse of notation) $\tilde{J}(l)=J(l)+3l-3=(\nu+3)l-3$ so that we still have $\tilde{J}(l)\simeq g/\hbar$. The arguments that rely on the smallness of g to allow us to use of Lemma (6.2) remain in force. We thus arrive at (6.27). We deal with it by using (10.3), exactly as above, and obtain exponential decay again in case $l=g/\hbar$. The long time estimates are also valid as the time dependence of the constants is unaltered. This shows that Theorems 3.1 and 3.3 are true with our generalized initial coherent states.

Theorem 3.2 also holds for these initial states provided we can control the sum in (7.3) with $J(l) = \nu l$. To do so, we first note that the last two factors of (7.3) can be bounded by $e^{\beta' J}$, for some β', so that they are of order $e^{g/\hbar}$. This is harmless if g is small enough because of the exponentially decreasing prefactor. Next, we use $k \leq l-1$ to obtain

$$\sqrt{(J+3k)!/(J!)} \;\leq\; (J+3k)^{3k/2}\,(J+3k)^{J/2}/\sqrt{J!} \;\leq\; c(\nu)\,\frac{((\nu+3)l)^{\nu l/2}}{(\nu l)^{\nu l/2}}\,(J+3k)^{3k/2},$$

for some constant $c(\nu)$. Thus, the sum in (7.3) is bounded by

$$c'(\nu)^l \sum_{k=0}^{l-1} C_2'^k\,\hbar^{k/2}\,(J+3k)^{3k/2}/k!, \tag{10.4}$$

for another constant $c'(\nu)$, and where C_2' is proportional to $C_0\,D_5$ in (7.3). Since

$$(J+3k)^{3k/2} \;\leq\; ((\nu+3)l)^{3k/2} \;\leq\; (((\nu+3)g)^{3/2}/\hbar^{3/2})^k,$$

we can bound (10.4) by

$$c'(\nu)^{g/\hbar}\,e^{C_2'((\nu+3)g)^{3/2}/\hbar}$$

which, again, is harmless for sufficiently small g.

To prove the validity of Theorem 3.4, insert (8.2) and (8.3) in the estimates above and check that the conclusion still holds. This is straightforward.

Finally, for Theorem 3.5 to hold, we first must consider the contribution associated to $\chi_1\,\xi_l$, which relies on (9.8). Here, (10.3) applies directly. Next, the first contribution from $\chi_2\xi_l$ is (9.11). It has the form (7.3) and yields exponential decay in the same way, for g small enough. It remains for us to bound (9.13). With $s \leq l+1+2k \leq 3l$, we use the estimate,

$$\sqrt{(J+s)!} \;\leq\; (\nu l+s)^{\nu l/2}\,(\nu l+s)^{s/2} \;\leq\; ((\nu+3)l)^{\nu l/2}\,((\nu+3)g/\hbar)^{s/2}$$

in (9.14). The first factor when multiplied by $e^{\tilde{\beta}J}/\sqrt{J!}$ is of order $e^{cg/\hbar}$ where c is independent of g. The final factor allows us to repeat the argument that led to (9.15). Hence, for g small enough, we get an exponentially small contribution in $\hbar$ and the result follows. ∎

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