Semiclassical Dynamics with Exponentially Small Error Estimates

George A. Hagedorn*
Department of Mathematics and
Center for Statistical Mechanics and Mathematical Physics
Virginia Polytechnic Institute and State University
Blacksburg, Virginia 24061-0123, U.S.A.

Alain Joye†
Institut Fourier
Unité Mixte de Recherche CNRS-UJF 5582
Université de Grenoble I
BP 74
F–38402 Saint Martin d'Hères Cedex, France

Abstract

We construct approximate solutions to the time–dependent Schrödinger equation

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

for small values of $\hbar$. If V satisfies appropriate analyticity and growth hypotheses and $|t|\le T$, these solutions agree with exact solutions up to errors whose norms are bounded by

$$C\;\exp\{\,-\,\gamma/\hbar\,\}\,,$$

for some C and $\gamma>0$. Under more restrictive hypotheses, we prove that for sufficiently small T', $|t|\le T'\,|\log(\hbar)|$ implies the norms of the errors are bounded by

$$C'\;\exp\{\,-\,\gamma'/\hbar^{\sigma}\,\}\,,$$

for some C', $\gamma'>0$, and $\sigma>0$.

*Partially Supported by National Science Foundation Grant DMS–9703751.
†Partially Supported by Fonds National Suisse de la Recherche Scientifique, Grant 8220-037200.

1 Introduction

In this paper, we construct exponentially accurate semiclassical approximations $\psi(x,\,t,\,\hbar)$ to certain normalized exact solutions $\Psi(x,\,t,\,\hbar)$ of the d–dimensional time–dependent Schrödinger equation

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

More precisely, our main result is that for $|t|\leq T$ and small values of $\hbar$, these approximations satisfy error estimates of the form

$$\|\,\psi(x,\,t,\,\hbar)\,-\,\Psi(x,\,t,\,\hbar)\,\|_{L^2(I\!\!R^d)}\;\leq\;C\;\exp\{\,-\,\gamma/\hbar\,\}\,, \tag{1.2}$$

where $\gamma>0$.

Our construction of $\psi(x,\,t,\,\hbar)$ is technically complicated, but quite explicit. It uses a particular collection of semiclassical wave packets $\{\,\varphi_j(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot\,)\,\}$ that are defined in [6], [7], and the next section. Here A and B are $d\times d$ complex matrices that satisfy certain conditions. The quantities a and η are elements of $I\!\!R^d$. For fixed A, B, $\hbar$, a, and η, $\{\,\varphi_j(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot\,)\,\}$ is an orthonormal basis of $L^2(I\!\!R^d)$ as j ranges over all d-dimensional multi-indices.

The function $\varphi_j(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot\,)$ is concentrated near position a, and its Fourier transform is concentrated near momentum η. Its position and momentum uncertainties are proportional to $\sqrt{\hbar}$. The position uncertainty is determined by the matrix $|A|=\sqrt{A\,A^*}$, and the momentum uncertainty is determined by $|B|=\sqrt{B\,B^*}$.

We construct $\psi(x,\,t,\,\hbar)$ by applying the idea of "optimal truncation" of an asymptotic expansion. For initial conditions of the form

$$\Psi(x,\,0,\,\hbar)\;=\;\sum_{|j|\leq J}\,c_j\,\varphi_j(A(0),B(0),\hbar,a(0),\eta(0),x), \tag{1.3}$$

with $\sum_{|j|\leq J}\,|c_j|^2\,=\,1$, there exist ([5], [6]) approximate solutions

$$\psi_l(x,\,t,\,\hbar)\;=\;e^{iS(t)/\hbar}\sum_{|j|\leq\widetilde{J}(l)}\,c_j(l,\,t,\,\hbar)\,\varphi_j(A(t),B(t),\hbar,a(t),\eta(t),x), \tag{1.4}$$

that satisfy

$$\sup_{t\in[-T,T]}\;\|\psi_l(x,\,t,\,\hbar)-\Psi(x,\,t,\,\hbar)\|_{L^2(I\!\!R^d)}\;\leq\;C(l)\,h^{l/2} \tag{1.5}$$

for some constant $C(l)$. Here $\widetilde{J}(l)\,=\,J+3l-3$, and $A(t)$, $B(t)$, $a(t)$, $\eta(t)$, and $S(t)$ are solutions to the classical equations of motion

$$\begin{array}{rcl}\dot a(t)&=&\eta(t),\\ \dot\eta(t)&=&-\,\nabla V(a(t)),\\ \dot A(t)&=&i\,B(t),\\ \dot B(t)&=&i\,V^{(2)}(a(t))\,A(t),\\ \dot S(t)&=&\dfrac{\eta(t)^2}{2}\,-\,V(a(t)),\end{array} \tag{1.6}$$

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

$$\begin{aligned} A^t(0)\,B(0)\;-\;B^t(0)\,A(0) &= 0, & (1.7)\\ A^*(0)\,B(0)\;+\;B^*(0)\,A(0) &= 2\,I. & (1.8)\end{aligned}$$

The $c_j(l,\,t,\,\hbar)$ satisfy a linear system of ordinary differential equations that we describe in the next section.

We carefully estimate the l–dependence of $C(l)$ in (1.5). Then, for each $\hbar$, we choose $l(\hbar)$ to minimize the error $C(l(\hbar))\,\hbar^{l(\hbar)/2}$ over all choices of l. It turns out that $l(\hbar)$ behaves like a constant times $1/\hbar$. We define $\psi(x,\,t,\,\hbar)=\psi_{l(\hbar)}(x,\,t,\,\hbar)$ and prove that (1.2) is satisfied.

For t in a fixed compact interval, the precise statement of our results is the following:

Theorem 1.1 *Suppose V is a real-valued function on $I\!R^d$ that is bounded below and has an analytic continuation to the set*

$$D\;=\;\{\,z\in \mathbb{C}^d\;:\;|Im\;z_j|\;<\;\delta,\;j=1,\,2,\,\cdots,\,d\,\}. \qquad (1.9)$$

Suppose further that there exist $M>0$ and $\tau>0$, such that

$$|\,V(z)\,|\;\le\;M\;\exp(\tau|z|^2),\qquad \textit{for all } z\in D, \qquad (1.10)$$

where $|z|^2\;=\;\sum_{j=1}^d\,|z_j|^2$. Suppose initial conditions $A(0)$, $B(0)$, $a(0)$, $\eta(0)$, $S(0)=0$, and c_j for $|j|\le J$ are specified that satisfy (1.7) and $\sum_{|j|\le J}\,|c_j|^2\;=\;1$. Then for any $T>0$, there exist C and $\gamma>0$, such that the difference between the semiclassical approximation $\psi(x,\,t,\,\hbar)$ and the exact solution $\Psi(x,\,t,\,\hbar)$ to the Schrödinger equation (1.1) with initial condition (1.3) satisfies

$$\|\,\psi(x,\,t,\,\hbar)\;-\;\Psi(x,\,t,\,\hbar)\,\|_{L^2(I\!R^d)}\;\le\;C\;\exp\{\,-\,\gamma/\hbar\,\}\,,$$

whenever $|t|\;\le\;T$.

Remarks 1. Theorem 1.1 can be generalized to allow time–dependent potentials. For example, suppose a potential $V(x,\,t)$ depends smoothly on t, is bounded below, and satisfies

$$\frac{1}{m!}\,|D^mV(x,\,t))|\;\le\;\frac{M\;\exp(\tau|x|^2)}{\delta^{|m|}},$$

for $|t|\le T$ for all multi-indices m. Suppose further that a classical solution $(a(t),\,\eta(t))$ to Newton's equations with potential $V(x,\,t)$ is bounded for $|t|\le T$. Then the conclusion to Theorem 1.1 holds.

2. Our results can also be extended to obtain weaker error estimates of the form $C\;\exp\{\,-\,\gamma/\hbar^\sigma\,\}$ for some $\sigma\in(0,\,1)$, when the potential belongs to a Gevrey class.

3. Theorem 1.1 is optimal in the sense that the conclusion fails if the hypotheses are relaxed slightly. For example, consider the one-dimensional potential $V(x)=\exp(-1/x^u)$, for $x>0$, and $V(x)=0$ for $x\le 0$, where $u>0$. It is shown in [8] that this potential belongs to the Gevrey class of order $1+1/u$. For initial conditions $a(0)=0$, $\eta(0)=0$, $A(0)=B(0)=1$,

$S(0) = 0$, and $c_j(0) = \delta_{j,0}$, our approximation yields $\varphi_0(1 + it, 1, \hbar, 0, 0)$, for all times. This function is very simple, and we can write the error term explicitly. By steepest descent analysis, we can show that there exist $\delta > 0$ and $\Sigma_1 > \Sigma_2 > 0$, such that $t \in (0, \hbar^{\delta})$ implies

$$\begin{aligned} \exp(-\Sigma_1/\hbar^{u/(1+u)}) \;&\leq\; \| \, e^{-itH(\hbar)/\hbar} \, \varphi_0(1, 1, \hbar, 0, 0, \cdot) \;-\; \varphi_0(1 + it, 1, \hbar, 0, 0, \cdot) \, \| \\ &\leq\; \exp(-\Sigma_2/\hbar^{u/(1+u)}). \end{aligned}$$

Note also that if we choose $a(0) = -a < 0$ and $\eta(0) = \eta > 0$, it is easy to check that the error term is $O(\exp(-\gamma/\hbar))$, for each $t < a/\eta$.

4. For all practical purposes, we can replace the c_j's by the corresponding Dyson expansion up to order $l(\hbar)$ without spoiling our exponential estimate. The normalization of the approximation, however, will be lost.

Theorem 1.1 can also be generalized to allow time intervals that grow like $|\log(\hbar)|$ as $\hbar$ tends to zero. However, we obtain a somewhat weaker conclusion. Our precise results are summarized by the following theorem.

Theorem 1.2 *Suppose V is bounded below and analytic in*

$$D \;=\; \{\, z \in \mathbb{C}^d \;:\; |Im\; z_j| \;<\; \delta,\; j = 1,\, 2,\, \cdots,\, d \,\}. \tag{1.11}$$

Suppose further that there exist $M > 0$ and $\tau > 0$, such that

$$|\, V(z) \,| \;\leq\; M\; \exp(\tau |z|), \qquad \text{for all } z \in D. \tag{1.12}$$

Suppose initial conditions $A(0)$, $B(0)$, $a(0)$, $\eta(0)$, $S(0) = 0$, and c_j for $|j| \leq J$ are specified that satisfy (1.7) and $\sum_{|j| \leq J} |c_j|^2 \;=\; 1$, and further assume there exist $N > 0$ and$\lambda > 0$, such that

$$\|A(t)\| \;\leq\; N\; \exp(\lambda |t|). \tag{1.13}$$

Then for sufficiently small $T' > 0$, there exist C', $\gamma' > 0$, and $\sigma > 0$, such that the difference between the semiclassical approximation $\psi(x,\, t,\, \hbar)$ and the exact solution $\Psi(x,\, t,\, \hbar)$ to the Schrödinger equation (1.1) with initial condition (1.3) satisfies

$$\| \, \psi(x,\, t,\, \hbar) \;-\; \Psi(x,\, t,\, \hbar) \, \|_{L^2(\mathbb{R}^d)} \;\leq\; C' \;\exp\{\, -\, \gamma'/\hbar^{\sigma} \,\},$$

whenever $|t| \;\leq\; T' \,|\log(\hbar)|$.

Remark Standard existence and uniqueness theorems for systems of ODE's show that condition (1.13) is satisfied if the norm of the Hessian $V^{(2)}(a(t))$ is uniformly bounded. That is the case if V is the sum of a quadratic polynomial plus a bounded analytic function. It is also the case if E denotes the energy of the considered trajectory and $\|V^{(2)}(x)\|$ is bounded on the connected component of the classically allowed region $D_E = \{x \in \mathbb{R}^d \,:\, V(x) \leq E\}$ that contains $a(t)$. This is satisfied for all confining potentials.

The propagation of coherent states is also considered by Combescure and Robert in [3], using an approximation given by a linear combination of squeezed states. (The squeezed states coincide with our semiclassical wave packets, although the notation is quite different.) Their emphasis is on the long time behavior of this approximation. The bound on the error term is of the form $C_l(t)\hbar^{l/2}$, with expicit control of the time-dependence of $C_l(t)$ in terms of classical quantities. The l behavior is however not investigated.

Results of a flavor similar to ours can be found in the work of Yajima [11]. They are obtained by means of the pseudo-differential techniques developed in the analytic context by Sjöstrand in [10]. These results concern the propagation of wave packets of the form $\varphi(x) = \mathrm{e}^{iS(x)/\hbar} f(x)$, where S is analytic and f belongs to the set of compactly supported Gevrey functions of order $s > 1$. Assuming the potential V is analytic, Yajima constructs approximations to the actual evolution of such wave packets that are valid up to an error, whose $L^2(I\!R^d)$ norm is of order $\mathrm{e}^{-\gamma/\hbar^{1/(2s-1)}}$, with $\gamma > 0$ (see Theorems 1.2, 1.2 and Lemma 2.5 in [11]). However, it should be possible to make use of the theory [10] to recover our results.

Similar issues have been dealt with by Bambusi, Graffi and Paul in [2]. They focus on the validity for large times of the semiclassical approximation of the Heisenberg evolution of a smooth observable, under analyticity assumptions on the hamiltonian. They prove that the semiclassical approximation remains useful for times up to order $|\ln(\hbar)|$, the Ehrensfest time scale. However, the Hamiltonians they can accomodate consist more or less of analytic perturbations of the harmonic oscillator that decay as x and p tend to infinity.

The paper is organized as follows: In the Section 2, we prove Theorem 1.1 under the assumption that two types of error terms satisfy certain bounds. We prove the two required bounds in Sections 3 and 4. In Section 5 we describe the proof of Theorem 1.2.

2 Proof of Theorem 1.1

We begin this section by presenting the definition of the semiclassical wave packets $\varphi_j(A,\, B,\, \hbar,\, a,\, \eta,\, x)$ that is given in [7]. A more explicit, but more complicated definition is given in [6]. Since [7] provides a detailed discussion of these wave packets, we do not prove all their properties here.

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 $|j| = \sum_{k=1}^d j_k$, $\quad j! = (j_1!)(j_2!)\cdots(j_d!)$, $x^j = x_1^{j_1} x_2^{j_2} \cdots x_d^{j_d}$, and $\displaystyle D^j = \frac{\partial^{|j|}}{(\partial x_1)^{j_1}(\partial x_2)^{j_2}\cdots(\partial x_d)^{j_d}}$.

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

$$A^t\, B \,-\, B^t\, A \;=\; 0, \tag{2.1}$$

$$A^*\, B \,+\, B^*\, A \;=\; 2\, I. \tag{2.2}$$

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 $\left(\mathrm{Re}\, BA^{-1}\right)^{-1} \;=\; A\, A^*$. We note that conditions (2.1) and (2.2) are preserved under the dynamics generated by (1.6).

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

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

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

$$\begin{aligned}\varphi_0(A,\, B,\, \hbar,\, a,\, \eta,\, x) \;&=\; \pi^{-d/4}\,\hbar^{-d/4}\,(\det(A))^{-1/2}\\ &\times\; \exp\Big\{-\langle\,(x-a),\, B\,A^{-1}\,(x-a)\,\rangle/(2\hbar) \;+\; i\,\langle\,\eta,\,(x-a)\,\rangle/\hbar\Big\}.\end{aligned} \tag{2.3}$$

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

$$\begin{aligned}\varphi_j(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot\,) \;&=\; \frac{1}{\sqrt{j!}}\;(\,\mathcal{A}_1(A,B,\hbar,a,\eta)^*)^{j_1}\;\;(\,\mathcal{A}_2(A,B,\hbar,a,\eta)^*)^{j_2}\;\cdots\\ &\times\;(\,\mathcal{A}_d(A,B,\hbar,a,\eta)^*)^{j_d}\;\;\varphi_0(A\,,B,\,\hbar,\,a,\,\eta,\,\cdot\,).\end{aligned}$$

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

2. For each A, B, $\hbar$, a, and η, the set $\{\,\varphi_j(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot\,)\,\}$ 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 [7] in the multi-dimensional case. If we set

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

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 [6], the state $\varphi_j(A,\, B,\, \hbar,\, a,\, \eta,\, x)$ is defined as a normalization factor times

$$\mathcal{H}_j(A;\, \hbar^{-1/2}\,|A|^{-1}\,(x-a))\;\varphi_0(A,\, B,\, \hbar,\, a,\, \eta,\, x).$$

Here $\mathcal{H}_j(A;\, y)$ is a $|j|^{\rm th}$ 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 the argument on page 370 of [6] or 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 $\varphi_j(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot\,)$ 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 $\varphi_0(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot\,)$ is determined by continuity in t after an arbitrary initial choice.

The proof of the theorem depends on the following abstract lemma.

Lemma 2.1 *Suppose $H(\hbar)$ is a family of self-adjoint operators for $\hbar > 0$. Suppose $\psi(t,\,\hbar)$ belongs to the domain of $H(\hbar)$, is continuously differentiable in t, and approximately solves the Schrödinger equation in the sense that*

$$i\,\hbar\,\frac{\partial\psi}{\partial t}(t,\,\hbar) \;=\; H(\hbar)\,\psi(t,\,\hbar) \;+\; \xi(t,\,\hbar), \tag{2.4}$$

where $\xi(t,\,\hbar)$ satisfies

$$\|\,\xi(t,\,\hbar)\,\| \;\leq\; \mu(t,\,\hbar). \tag{2.5}$$

Then, for $t>0$,

$$\|\,e^{-itH(\hbar)/\hbar}\,\psi(0,\,\hbar) \;-\; \psi(t,\,\hbar)\,\| \;\leq\; \hbar^{-1}\,\int_0^t\,\mu(s,\,\hbar)\,ds. \tag{2.6}$$

The analogous statement holds for $t<0$.

Proof: Assume $t>0$; the proof for $t<0$ is similar. By the unitarity of the propagator $\mathrm{e}^{-itH(\hbar)/\hbar}$ and the fundamental theorem of calculus, the quantity on the left-hand side of (2.6) can be estimated as follows:

$$\begin{aligned}
&\|\,\mathrm{e}^{-itH(\hbar)/\hbar}\,\psi(0,\,\hbar) \;-\; \psi(t,\,\hbar)\,\| \\
=\;& \|\,\psi(0,\,\hbar) \;-\; \mathrm{e}^{itH(\hbar)/\hbar}\,\psi(t,\,\hbar)\,\| \\
=\;& \|\,\int_0^t\,\frac{\partial}{\partial s}\,\Big(\psi(0,\,\hbar) \;-\; \mathrm{e}^{isH(\hbar)/\hbar}\,\psi(s,\,\hbar)\Big)\;ds\,\| \\
=\;& \|\,\int_0^t\,\left(-i\,\hbar^{-1}\,\mathrm{e}^{isH(\hbar)/\hbar}\,H(\hbar)\,\psi(s,\,\hbar) \;-\; \mathrm{e}^{isH(\hbar)/\hbar}\,\frac{\partial\psi}{\partial s}(s,\,\hbar)\right)\;ds\,\| \\
=\;& \|\,\int_0^t\,i\,\hbar^{-1}\,\mathrm{e}^{isH(\hbar)/\hbar}\,\xi(s,\,\hbar)\;ds\,\| \\
\leq\;& \hbar^{-1}\,\int_0^t\,\mu(s,\hbar)\,ds.
\end{aligned}$$

This proves the lemma. ■

Because V is smooth and bounded below, there exist global solutions to the first two equations of the system (1.6) for any initial condition. It then follows immediately that the remaining three equations of the system (1.6) have global solutions. Furthermore, it is not difficult ([5], [6]) to prove that (2.1) and (2.2) are preserved by the flow.

As mentioned in the introduction, it is proved in [5] and [6] that initial conditions of the form (1.3) give rise to approximate solutions of the form

$$\psi_l(x,\, t,\, \hbar) \;=\; e^{iS(t)/\hbar} \sum_{|j|\le \widetilde{J}(l)} c_j(l,\, t,\, \hbar)\, \varphi_j(A(t), B(t), \hbar, a(t), \eta(t), x),$$

with errors whose norms are of order $\hbar^{l/2}$. Here $\widetilde{J}(l) = J + 3l - 3$, and $A(t)$, $B(t)$, $a(t)$, $\eta(t)$, and $S(t)$ satisfy (1.6). The coefficients $c_j(l,\, t,\, \hbar)$ satisfy the linear system

$$i\,\hbar\, \dot{c}_k(l,\, t,\, \hbar) \;=\; \sum_{|j|\le \widetilde{J}(l)} K_{k\,j}(l,\, t,\, \hbar)\, c_j(l,\, t,\, \hbar), \qquad\qquad |k| = 0,\, 1,\, \dots,\, \widetilde{J}(l), \tag{2.7}$$

with initial conditions $c_j(l,\, 0,\, \hbar) = c_j$, for $|j| \le J$ in accordance with (1.3) and $c_j(l,\, 0,\, \hbar) = 0$ for $|j| > J$.

To specify the $(J+3l-2) \times (J+3l-2)$ matrix $K(l,\, t,\, \hbar)$ that appears in (2.7), we first decompose the potential as

$$V(x) = W_a(x) + Z_a(x) \equiv W_a(x) + (V(x) - W_a(x)), \tag{2.8}$$

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

$$W_a(x) \;\equiv\; V(a) \;+\; V^{(1)}(a)\, (x-a) \;+\; V^{(2)}(a)\, (x-a)^2/2, \tag{2.9}$$

Next (reverting to multi-index notation), we approximate $Z_a(x)$ by its Taylor approximation of order $l+1$,

$$Z_a^{[l]}(x) \;=\; \sum_{3\le|m|\le l+1} \frac{(D^m V)(a)}{m!}\, (x-a)^m, \tag{2.10}$$

and define the infinite matrix

$$\begin{aligned}&\widetilde{K}_{k\,j}(l,\, t,\, \hbar) \;=\\ &\langle\, \varphi_k(A(t), B(t), \hbar, a(t), \eta(t), x),\;\; Z_{a(t)}^{[l]}(x)\, \varphi_j(A(t), B(t), \hbar, a(t), \eta(t), x)\,\rangle.\end{aligned} \tag{2.11}$$

Then, we obtain the matrix $K(l,\, t,\, \hbar)$ from $\widetilde{K}(l,\, t,\, \hbar)$ by restricting the indices to $|j| \le \widetilde{J}(l)$ and $|k| \le \widetilde{J}(l)$.

The general strategy [5], [6], [7] to show that $\psi_l(x,\, t,\, \hbar)$ is an approximation to the actual solution $\Psi(x,\, t,\, \hbar)$ of (1.1) and (1.3) up to order $\hbar^{l/2}$ is as follows: From [7], we know that for all multi-indices j,

$$\begin{aligned}&i\,\hbar\, \frac{\partial}{\partial t}\, \left[\mathrm{e}^{iS(t)/\hbar}\, \varphi_j(A(t), B(t), \hbar, a(t), \eta(t), x)\right]\\ =\;& \left(-\,\frac{\hbar^2}{2}\,\Delta \;+\; W_{a(t)}(x)\right)\, \left[\mathrm{e}^{iS(t)/\hbar}\, \varphi_j(A(t), B(t), \hbar, a(t), \eta(t), x)\right].\end{aligned} \tag{2.12}$$

Thus, the φ_j take into account the kinetic energy and $W_{a(t)}(x)$ parts of the Hamiltonian. Next, we expand the exact solution as

$$\Psi(x,\,t,\,\hbar) \;=\; \sum_j\, b_j(\hbar,\,t)\, \mathrm{e}^{iS(t)/\hbar}\, \varphi_j(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, x),$$

where the $b_j(\hbar,\,t)$ satisfy an infinite linear system of ordinary differential equations whose matrix is obtained from the $Z_{a(t)}(x)$ term in the Hamiltonian. In that system, we make a first approximation by replacing the function $Z_{a(t)}(x)$ by its Taylor approximation $Z^{[l]}_{a(t)}(x)$. This yields an infinite linear system whose matrix is $\widetilde{K}(l,\,t,\,\hbar)$. Its entries are time dependent polynomials in $\hbar^{1/2}$ of order $l-1$. We make a second approximation by truncating the infinite system to obtain (2.7) that is satisfied by the $c_j(l,\,t,\,\hbar)$. The result (1.5) is proved by using Lemma 2.1 to show that the errors generated by the Taylor approximation and the truncation approximation are of order $\hbar^{l/2}$.

As described in the introduction, we construct the exponentially accurate approximate solution $\psi(x,\,t,\,\hbar) \;=\; \psi_{l(\hbar)}(x,\,t,\,\hbar)$, by keeping track of the l–dependence of $C(l)$ in (1.5) and then choosing $l(\hbar)$ in order to minimize the error.

In the remainder of this section, we prove Theorem 1.1 under the assumption that the following three technical lemmas are true. We prove the first lemma in Section 3. It estimates errors that arise from our replacement of $Z_{a(t)}(x)$ by $Z^{[l]}_{a(t)}(x)$. The second and third lemmas are proved in Section 4. They bound certain matrix elements and combinatorial quantities that arise from the truncation approximation discussed above.

Lemma 2.2 *Suppose V satisfies the hypotheses of Theorem 1.1, $|m|=l+2$, $\widetilde{J}(l)=J+3l-3$, and*

$$\psi_l(x,\,t,\,\hbar) \;=\; e^{iS(t)/\hbar} \sum_{|j|\le\widetilde{J}(l)} c_j(l,\,t,\,\hbar)\, \varphi_j(A(t), B(t), \hbar, a(t), \eta(t), x),$$

with $\sum_{|j|\le\widetilde{J}(l)}\, |c_j(l,\,t,\,\hbar)|^2 \;=\; 1$.
Let $\zeta(x,a(t)) = (a(t)+\theta_{x,a(t)}(x-a(t))) \in I\!\!R^d$, with $\theta_{x,a(t)}\in(0,\,1)$. There exist constants g_0 and g_1, that depend on d and J only, such that for sufficiently small $\hbar$,

$$\begin{aligned}
&\left\|\, \frac{D^mV(\zeta(x,a(t)))}{m!}\;(x-a(t))^m\;\psi_l(\cdot,\,t,\,\hbar)\,\right\| \\
&\le\; g_0\,M\,\exp(4\tau(\delta^2d+a(t)^2))\,\left(g_1\,\sqrt{\hbar(l+2)}\,\|A(t)\|/\delta\right)^{l+2}.
\end{aligned} \tag{2.13}$$

Lemma 2.3 *We define the infinite matrix*

$$\begin{aligned}
&\widetilde{X}^m_{j\,k}(t,\,\hbar) \;= \\
&\langle\, \varphi_j(A(t), B(t), \hbar, a(t), \eta(t), \cdot),\; (x-a(t))^m\, \varphi_k(A(t), B(t), \hbar, a(t), \eta(t), \cdot)\,\rangle,
\end{aligned} \tag{2.14}$$

and then define the finite matrix $X^m(l,\,t,\,\hbar)$ from $\widetilde{X}^m(t,\,\hbar)$ by restricting its indices to $|j|\le\widetilde{J}(l)$ and $|k|\le\widetilde{J}(l)$. Then, $X^m_{j\,k}(l,\,s,\,\hbar)=0$ and $\widetilde{X}^m_{j\,k}(s,\,\hbar)=0$ if $\Big||j|-|k|\Big| > |m|$ and, *for each $N > 0$, there exists $D(N) < \infty$, such that*

$$\sup_{\substack{|k| \,\leq \widetilde{J}(l) \\ \widetilde{J}(l)+1 \,\leq\, |j| \,\leq \widetilde{J}(l)+l+1}} \left| \left(\widetilde{X}^{m_0}(t_0,\hbar) X^{m_1}(l,t_1,\hbar) X^{m_2}(l,t_2,\hbar) \cdots X^{m_q}(l,t_q,\hbar) \right)_{j\,k} \right|$$

$$\leq \quad \left(D(N) \sqrt{\hbar\, \widetilde{J}(l)} \sup_{t \in \{t_0,t_1,t_2,\cdots t_q\}} \|A(t)\| \right)^{|m_0|+|m_1|+|m_2|\cdots+|m_q|}, \tag{2.15}$$

for any collection $m_0,\, m_1,\, \ldots,\, m_q$ of multi-indices that satisfy $|m_j|/\widetilde{J}(l) \leq N$.

Lemma 2.4 *We define*

$$F_p(n,\,q) \;=\; \sum_{\substack{1 \,\leq\, |m_1|,|m_2|,\cdots,|m_q| \,\leq\, p \\ |m_1|+|m_2|+\cdots+|m_q| \,=\, n}} 1 \tag{2.16}$$

to be the number of distinct sets $\{\, m_1,\, m_2,\, \ldots,\, m_q \,\}$, where each m_j is a d–dimensional multi-index with $1 \leq |m_j| \leq p$ and $|m_1|+|m_2|+\cdots+|m_q| = n$. We note that $F_p(n,\,q)$ is zero unless $q \leq n \leq qp$. Suppose that a function $L_q(l)$ satisfies

$$L_q(l) \;\leq\; \frac{C_1^q}{\hbar^q\, q!} \sum_{n=3l-2}^{q(l+1)} (C_2 \hbar l)^{n/2}\, F_{l+1}(n,\,q), \tag{2.17}$$

where C_1 and C_2 are constants. Let $[\![\, \alpha \,]\!]$ denote the greatest integer less than or equal to α. Then there exists $g^* > 0$, such that for any $g \in (0,\, g^*)$, there exist positive constants C_3, γ_1, and $\hbar^*$, that depend only on g, C_1, and C_2, such that

$$0 < \hbar < \hbar^*, \quad l(\hbar) \;=\; [\![\, g/\hbar \,]\!], \quad \textit{and} \quad 2 \leq q \leq l(\hbar)+2 \tag{2.18}$$

imply

$$L_q(l(\hbar)) \;\leq\; C_3 \, \exp\{\,-\gamma_1/\hbar\,\}\,. \tag{2.19}$$

Proof of Theorem 1.1: We define $\psi_l(x,\,t,\,\hbar)$ by (1.4), where the $c_j(l,\,t,\,\hbar)$ are determined by the system (2.7) and initial conditions described above.

To apply Lemma 2.1 we define

$$\xi_l(x,\,t,\,\hbar) \;=\; i\,\hbar\, \frac{\partial}{\partial t} \psi_l(x,\,t,\,\hbar) \;-\; \left(-\,\frac{\hbar^2}{2}\, \Delta \;+\; V(x) \right)\, \psi_l(x,\,t,\,\hbar). \tag{2.20}$$

By using (2.12), we see that this can be decomposed as a sum of two terms,

$$\xi_l^{(1)}(x,\,t,\,\hbar) \;\;=\;\; \left(Z_{a(t)}^{[l]}(x) \;-\; Z_{a(t)}(x) \right)\, \psi_l(x,\,t,\,\hbar) \tag{2.21}$$

and

$$\xi_l^{(2)}(x,\,t,\,\hbar) \;\;=\;\; -\,P_{\{|j| \geq l+2\}}\, Z_{a(t)}^{[l]}(x)\, \psi_l(x,\,t,\,\hbar), \tag{2.22}$$

where $P_{\{|j|\geq l+2\}}$ is the orthogonal projection onto the span of the set $\{\,\varphi_j(A(t),\,B(t),\,\hbar,\,a(t),\,\eta(t),\,\cdot\,):\ \ |j|\geq l+2\,\}$.

By the standard Taylor series error formula,

$$Z_{a(t)}(x)\ -\ Z_{a(t)}^{[l]}(x)\ =\ \sum_{|m|=l+2}\frac{D^mV(\zeta(x,a(t)))}{m!}\,(x-a(t))^m,$$

for some $\zeta(x,a)=(a+\theta_{x,a}(x-a))$, with $\theta_{x,a}\in(0,\,1)$. Thus, by the crude estimate

$$\begin{aligned}\sum_{|m|=n}1\ \leq\ \sum_{|m|\leq n}1\ &\leq\ \sum_{j=1}^{d}\sum_{m_j\leq n}1\\ &=\ (n+1)^d\ =\ \mathrm{e}^{d\,\ln(n+1)}\ \leq\ \left(\mathrm{e}^d\right)^n,\end{aligned}\tag{2.23}$$

and Lemma 2.2, we obtain

$$\begin{aligned}&\left\|\,\xi_l^{(1)}(\cdot,\,t,\,\hbar)\,\right\|\\ \leq\ &\sum_{|m|=l+2}\left\|\frac{D^mV(\zeta(x,a(t)))}{m!}\,(x-a(t))^m\ \psi_l(\cdot,\,t,\,\hbar)\right\|\\ \leq\ &g_0\,M\,\exp(4\tau(\delta^2d+a(t)^2))\,\left(g_1\,\sqrt{\hbar(l+2)}\,\|A(t)\|/\delta\right)^{l+2}\,\left(\mathrm{e}^d\right)^{l+2}.\end{aligned}$$

Thus, there exist constants C_4 and C_5, such that $|t|\ \leq\ T$ implies

$$\left\|\,\xi_l^{(1)}(\cdot,\,t,\,\hbar)\,\right\|\ \leq\ C_4\,\left(C_5\,\sqrt{\hbar(l+2)}\right)^{l+2}.\tag{2.24}$$

The quantity $\xi_l^{(2)}(\cdot,\,t,\,\hbar)$ satisfies

$$\langle\,\varphi_j(A(t),B(t),\hbar,a(t),\eta(t),x),\ \xi_l^{(2)}(x,\,t,\,\hbar)\,\rangle\ =\ 0,\quad\text{if}\quad\begin{cases}0\leq|j|\leq\widetilde{J}(l)&\text{or}\\|j|>\widetilde{J}(l)+l+1,&\end{cases}$$

and

$$\begin{aligned}&\langle\,\varphi_j(A(t),B(t),\hbar,a(t),\eta(t),x),\ \xi_l^{(2)}(x,\,t,\,\hbar)\,\rangle\ =\\ &\sum_{|k|\leq\widetilde{J}(l)}\langle\,\varphi_j(A(t),B(t),\hbar,a(t),\eta(t),x),\ Z_{a(t)}(x)\,\varphi_k(A(t),B(t),\hbar,a(t),\eta(t),x)\,\rangle\,c_k(t)\\ &=(\widetilde{K}(t)\,\mathbf{c}(t))_j,\qquad\text{if}\quad\widetilde{J}(l)<|j|\leq\widetilde{J}(l)+l+1,\end{aligned}\tag{2.25}$$

where we denote the $c_j(l,\,t,\,\hbar)$ collectively by the vector $\mathbf{c}(l,\,t,\,\hbar)$. We easily verify these facts by using (2.7), (2.11), (2.12) and Lemma 2.3. To estimate the norm of $\xi_l^{(2)}(\cdot,\,t,\,\hbar)$, we use the Dyson expansion with remainder to decompose

$$\mathbf{c}(l,\,t,\,\hbar)=\sum_{q=0}^{l}\mathbf{c}^q(l,\,t,\,\hbar)\ +\ \mathbf{r}(l,\,t,\,\hbar),\tag{2.26}$$

where (dropping some arguments)

$$\mathbf{c}^q(t) = \int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{q-1}} ds_q (i\hbar)^{-q} K(s_1) K(s_2) \cdots K(s_q)\, \mathbf{c}(0), \tag{2.27}$$

and

$$\mathbf{r}(t) = \int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_l} ds_{l+1} (i\hbar)^{-(l+1)} K(s_1) K(s_2) \cdots K(s_{l+1})\, \mathbf{c}(s_{l+1}). \tag{2.28}$$

Using (2.11), (2.10), and (2.14), we see that each $\mathbf{c}^q(l,\, t,\, \hbar)$ is of order $\hbar^{q/2}$ and that $\mathbf{r}(l,\, t,\, \hbar)$ is of order $\hbar^{(l+1)/2}$.

To estimate the norm of $\xi_l^{(2)}(\cdot,\, t,\, \hbar)$ we study the j^{th} component of $\widetilde{K}(t)\mathbf{c}(l,\, t,\, \hbar)$, with $|j| > \widetilde{J}(l)$. Because of (2.26), this coefficient is a sum of two types of terms: those that arise from $\mathbf{c}^q(l,\, t,\, \hbar)$ and those that arise from $\mathbf{r}(l,\, t,\, \hbar)$. Using (2.10), we expand $K(l,\, t,\, \hbar)$ in (2.27) and (2.28) and $\widetilde{K}(l,\, t,\, \hbar)$ in terms of $X^m(l,\, t,\, \hbar)$ and $\widetilde{X}^m(t,\, \hbar)$, to obtain

$$\begin{aligned} \widetilde{K}(t)\mathbf{c}^q(t) = (i\hbar)^{-q} & \sum_{n=3(q+1)}^{(l+1)(q+1)} \sum_{\substack{m_0,\, m_1,\, m_2,\, \cdots,\, m_q \\ |m_0| + |m_1| + \cdots + |m_q| = n \\ 3 \le |m_j| \le l+1}} \\ & \int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{q-1}} ds_q \frac{D^{m_0} V(a(t)) D^{m_1} V(a(s_1)) \cdots D^{m_q} V(a(s_q))}{m_0! m_1! m_2! \cdots m_q!} \\ & \qquad \times\, \widetilde{X}^{m_0}(t) X^{m_1}(s_1) X^{m_2}(s_2) \cdots X^{m_q}(s_q)\, \mathbf{c}(0), \end{aligned} \tag{2.29}$$

and

$$\begin{aligned} \widetilde{K}(t)\mathbf{r}(t) = (i\hbar)^{-(l+1)} & \sum_{n=3(l+2)}^{(l+1)(l+2)} \sum_{\substack{m_0,\, m_1,\, m_2,\, \cdots,\, m_{l+1} \\ |m_0| + |m_1| + \cdots + |m_{l+1}| = n \\ 3 \le |m_j| \le l+1}} \\ & \int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_l} ds_{l+1} \frac{D^{m_0} V(a(t)) D^{m_1} V(a(s_1)) \cdots D^{m_{l+1}} V(a(s_{l+1}))}{m_0! m_1! m_2! \cdots m_{l+1}!} \\ & \qquad \times\, \widetilde{X}^{m_0}(t) X^{m_1}(s_1) X^{m_2}(s_2) \cdots X^{m_{l+1}}(s_{l+1})\, \mathbf{c}(s_{l+1}). \end{aligned} \tag{2.30}$$

The values of m_j that occur in both (2.29) and (2.30) satisfy

$$|m_j|/\widetilde{J}(l) \le (l+1)/(3l-3) \le 1, \tag{2.31}$$

as long as $l \ge 3$. So, we can apply Lemma 2.3 with $N = 1$.

Recall that $X^m_{j\,k}(l,\, s,\, \hbar) = 0$ and $\widetilde{X}^m_{j\,k}(s,\, \hbar) = 0$ if $\Big||j| - |k|\Big| > |m|$. Since $c_k(0)$ is non-zero only for $|k| \le J$, and we need only consider the j^{th} coefficient of $\widetilde{K}(t)\mathbf{c}(t)$ for $|j| > \widetilde{J}(l)$, the only relevant values of n in (2.29) must satisfy

$$n \ge 3l - 2. \tag{2.32}$$

This condition is also satisfied for all values of n in (2.30), since the sum begins with $n = 3l+6$.

To use the analyticity assumptions to get estimates on the derivatives of V, 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 $z \in C_\delta(a(t))$, then, for all $j = 1, 2, \cdots, d$,

$$|z_j| \leq \delta + |a_j(t)|.$$

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

$$\frac{1}{m!}\,|D^m V(a(t))| \;\leq\; \frac{\sup_{z \in C_\delta(a(t))} |V(z)|}{\delta^{|m|}} \;\equiv\; \frac{v(t)}{\delta^{|m|}} \tag{2.33}$$

where

$$v(t) \;\leq\; M\ \exp(4\tau(\delta^2 d + a^2(t))).$$

Furthermore, since $\|A(t)\|$ depends continuously on t, there exists $w(T)$, such that

$$\sup_{t \in [-T,T]}\ \|A(t)\| \;\leq\; w(T).$$

The norm of the vector $\mathbf{c}(t)$ is 1 since $K(l,\, t,\, \hbar)$ is self-adjoint. Thus, the non-zero entries of $\mathbf{c}(0)$ are each bounded by 1, and by a crude estimate, there are at most $(J+1)^d$ of them. Similarly, $\mathbf{c}(t)$ has at most $(\widetilde{J}(l)+1)^d$ non-zero entries, each of which is bounded by 1. Thus, for $l \geq 3$, (2.11), (2.10), (2.14), (2.29), (2.30), (2.32), (2.31), and Lemma 2.3 imply the following two estimates when j satisfies $\widetilde{J}(l) + 1 \leq |j| \leq \widetilde{J}(l) + l + 1$:

$$\begin{aligned}
&\left|\, (\widetilde{K}(t)\, \mathbf{c}^q(t))_j \,\right| \\
\leq\;& v(t) \frac{\left(\int_0^T v(s)\, ds\right)^q}{\hbar^q q!} \sum_{n=3l-2}^{(l+1)(q+1)} (D(1)\, w(T)/\delta)^n\, \hbar^{n/2}\, \widetilde{J}(l)^{n/2}\, F_{l+1}(n, q+1)\, (J+1)^d \\
=\;& \frac{v(t)\hbar(q+1)(J+1)^d}{\int_0^T v(s)ds} \frac{\left(\int_0^T v(s)ds\right)^{q+1}}{\hbar^{q+1}(q+1)!} \sum_{n=3l-2}^{(l+1)(q+1)} (D(1)w(T)\sqrt{\hbar \widetilde{J}(l)}/\delta)^n F_{l+1}(n, q+1)
\end{aligned} \tag{2.34}$$

and

$$\begin{aligned}
&\left|\, (\widetilde{K}(t)\mathbf{r}(t))_j \,\right| \\
\leq\;& \frac{v(t)\hbar(l+2)(\widetilde{J}(l)+1)^d}{\int_0^T v(s)ds} \frac{\left(\int_0^T v(s)ds\right)^{l+2}}{\hbar^{l+2}(l+2)!} \sum_{n=3l-2}^{(l+1)(l+2)} (D(1)w(T)\sqrt{\hbar \widetilde{J}(l)}/\delta)^n F_{l+1}(n, l+2),
\end{aligned} \tag{2.35}$$

where $F_p(n, q)$ is defined by (2.16).

By Lemma 2.4, (2.34), and (2.35), both $\left|\,(\widetilde{K}(t)\,\mathbf{c}^q(t))_j\,\right|$ and $\left|\,(\widetilde{K}(t)\mathbf{r}(t))_j\,\right|$ are bounded by $C_3\,\exp\,\{\,-\gamma_1/\hbar\,\}$ for an appropriate choice of $l(\hbar)\;=\;[\![\,g/\hbar\,]\!]$ and sufficiently small $\hbar$. Each of the $l+2$ terms in (2.26) contributes a term of this type to $\xi_l^{(2)}(x,\,t,\,\hbar)$, so

$$\begin{aligned}\hbar^{-1}\;\left\|\,\xi_l^{(2)}(x,\,t,\,\hbar)\,\right\| \;&\leq\; C_3\,\hbar^{-1}\,(l(\hbar)+2)\,\exp\,\{\,-\,\gamma_1/\hbar\,\}\\ &\leq\; C_3\,\exp\,\{\,-\,\gamma_2/\hbar\,\}\,,\end{aligned}$$

for any $\gamma_2<\gamma_1$ when $\hbar$ is sufficiently small.

We shrink g if necessary to make

$$C_5^2\,g<1 \tag{2.36}$$

and set $l=l(\hbar)$ in (2.24). This yields a similar estimate

$$\hbar^{-1}\;\left\|\,\xi_l^{(1)}(\cdot,\,t,\,\hbar)\,\right\|\;\leq\;C_6\,\exp\,\{\,-\,\gamma_3/\hbar\,\}\,,$$

for some $\gamma_3>0$.

We combine these two estimates and apply Lemma 2.1 to obtain (1.2) with $\gamma\;=\;\min\,\{\gamma_2,\,\gamma_3\}$. This proves the theorem. ■

3 Proof of Lemma 2.2

For simplicity, we drop the t dependence in the notation throughout this section.

To prove Lemma 2.2, we use Hölder's inequality to see that $\sum_{|j|\leq\widetilde{J}(l)}\,|c_j(l,\,\hbar)|^2\;=\;1$ implies

$$\begin{aligned}\sum_{|j|\leq\widetilde{J}(l)}\;|c_j(l,\,\hbar)|\;&\leq\;\left(\sum_{|j|\leq\widetilde{J}(l)}\;|c_j(l,\,\hbar)|^2\right)^{1/2}\;\left(\sum_{|j|\leq\widetilde{J}(l)}\;1\right)^{1/2}\\ &\leq\;\left(\widetilde{J}(l)+1\right)^{d/2}.\end{aligned}$$

Thus, it is sufficient to prove

$$\begin{aligned}&\left\|\,\frac{D^mV(\zeta(x,a))}{m!}\;(x-a)^m\;\varphi_j(A,\,B,\,\hbar,\,a,\,\eta,\,x)\,\right\|\\ &\leq\;g_3\,M\,\exp(4\tau(\delta^2d+a^2))\;\left(g_4\,\sqrt{\hbar(l+2)}\,\|A\|/\delta\right)^{l+2},\end{aligned} \tag{3.1}$$

for some g_3 and g_4, whenever $|j|\leq\widetilde{J}(l)$.

We mimic the proof of 2.33 to obtain a bound on $D^mV(\zeta(x,a))/m!$. 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

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

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

$$\frac{1}{m!}\,|D^m V(\zeta(x,a))| \leq M\ \frac{\exp(4\tau(\delta^2 d + a^2))}{\delta^{|m|}}\ \exp(2\tau(x-a)^2). \tag{3.2}$$

Thus, estimate (3.1) follows from the corresponding estimate on the integral

$$I = \int_{I\!R^d} (x-a)^{2m}\ \exp(4\tau(x-a)^2)\ |\varphi_j(A,\, B,\, \hbar,\, a,\, \eta,\, x)|^2\, dx. \tag{3.3}$$

Performing the change of variables $x \mapsto y = |A|^{-1}(x-a)/\hbar^{1/2}$, and using the explicit formula for φ_j, we see that

$$I\ =\ \frac{\hbar^{|m|}}{2^{|j|}\, j!\, \pi^{d/2}}\ \int_{I\!R^d} (|A|y)^{2m}\ \exp(-y^2 + 4\tau\hbar(|A|y)^2)\ |\mathcal{H}_j(A;\, y)|^2\, dy, \tag{3.4}$$

where $\mathcal{H}_l(A;\, y)$ is the polynomial described in Remarks 4 and 5 that immediately follow the definition of $\varphi_j(A, B, \hbar, a, \eta, x)$ in Section 2.

We assume henceforth that $\hbar$ is sufficiently small that

$$4\,\tau\,\hbar\,\|A\|^2\ \leq\ 1/2. \tag{3.5}$$

The estimate $(|A|y)^2\ \leq\ \|A\|^2\, y^2$ implies $(|A|y)_k^2\ \leq\ \|A\|^2\, y^2$, for $k = 1, 2, \cdots, d$. From this, we conclude

$$I\ \leq\ \frac{(\hbar\,\|A\|^2)^{|m|}}{2^{|j|}\, j!\, \pi^{d/2}}\ \int\ y^{2|m|}\ \exp(-y^2/2)\,|\mathcal{H}_j(A;\, y)|^2\, dy. \tag{3.6}$$

We next need an estimate on $|\mathcal{H}_j(A;\, y)|$. By Remark 5 after the definition in Section 2,

$$\left(-\Delta + y^2\right)\ \mathcal{H}_j(A;\, y)\, \mathrm{e}^{-y^2/2} = (2|j| + d)\ \mathcal{H}_j(A;\, y)\, \mathrm{e}^{-y^2/2}. \tag{3.7}$$

This equation states that $\mathcal{H}_j(A;\, y)\, \mathrm{e}^{-y^2/2}$ is a eigenfunction of $-\Delta + y^2$ corresponding to the eigenvalue $2|j| + d$. Introducing normalization factors, we conclude that

$$2^{-|j|/2}\,(j!)^{-1/2}\,\pi^{-d/4}\,\mathcal{H}_j(A;\, y)\, \mathrm{e}^{-y^2/2}\ =\ \sum_{|k|=|j|}\ b_k\,\varphi_{k_1}(y_1)\varphi_{k_2}(y_2)\cdots\varphi_{k_d}(y_d), \tag{3.8}$$

where $\varphi_k(y)\ =\ 2^{-k/2}\,(k!)^{-1/2}\,\pi^{-1/4}\,H_k(y)\,\mathrm{e}^{-y^2/2}$ is the normalized eigenfunction of $-\frac{\partial^2}{\partial y^2} + y^2$ corresponding to the eigenvalue $2k+1$, and the coefficients b_k satisfy $\sum_{|k|=|j|}\,|b_k|^2\ =\ 1$. We can thus deduce an estimate of $\mathcal{H}_j(A;\, y)$ from an estimate for usual Hermite polynomials $H_k(y)$:

$$\begin{aligned} |\mathcal{H}_j(A;\, y)|^2\ &=\ |\sum_{|k|=|j|}\ b_k\, H_{k_1}(y_1)H_{k_2}(y_2)\cdots H_{k_d}(y_d)|^2 \\ &\leq\ \sum_{|k|=|j|}\ |H_{k_1}(y_1)H_{k_2}(y_2)\cdots H_{k_d}(y_d)|^2. \end{aligned} \tag{3.9}$$

The Hermite polynomials, in turn, satisfy the following bounds.

Lemma 3.1 *If $|y| > \sqrt{2k+1}$, then*

$$|H_k(y)| \;\leq\; 2^k\,|y|^k, \tag{3.10}$$

and there exists a numerical constant $\kappa > 0$, such that for all $y \in I\!R$,

$$|H_k(y)| \;\leq\; \kappa\, 2^{k/2}\,\sqrt{k!}\; e^{y^2/2}. \tag{3.11}$$

Proof: The second statement is well known. See [1], formula 22.14.17 or [4], formula 8.954.2.

By symmetry, it is sufficient to prove (3.10) for $y > 0$. It is well known that the k^{th} eigenfuction of the harmonic oscillator is non-zero in the classically forbidden region $|y| > \sqrt{2k+1}$. It is also well known that $H_k(y) = 2^k y^k + P_k(y)$ where $P_k(y)$ is a polynomial of degree $k-2$. Thus, we have

$$H_k(y)/(2^k y^k) = 1 + B_k(y),$$

where B_k satisfies

$$B_k(y) \;=\; O(1/y^2) \qquad \text{for large } y,$$

and

$$B_k(y) > -1 \qquad \text{if} \quad y > \sqrt{2k+1}.$$

Using standard properties of the Hermite polynomials, we see that

$$\begin{aligned}
B_k'(y) \;&=\; (y\,H_k'(y) \;-\; k\,H_k(y))/(2^k\,y^{k+1}) \\
&=\; (2\,k\,y\,H_{k-1}(y) \;-\; k\,H_k(y))/(2^k\,y^{k+1}) \\
&=\; k\,(2\,y\,H_{k-1}(y) \;-\; (2\,y\,H_{k-1}(y) \;-\; 2\,(k-1)\,H_{k-2}(y)))/(2^k\,y^{k+1}) \\
&=\; k\,(k-1)\,H_{k-2}(y)/(2^{k-1}\,y^{k+1}).
\end{aligned}$$

So, if $y > \sqrt{2k+1}$, we see that $B_k'(y) > 0$. Thus, $y > \sqrt{2k+1}$ implies $-1 < B_k(y) < 0$, which implies (3.10). ∎

In (3.6), we use the multinomial expansion

$$(y^2)^{|m|} \;=\; \sum_{|n|=|m|} \begin{pmatrix} & |m| & \\ n_1 & \cdots & n_d \end{pmatrix} y_1^{2n_1}\,y_2^{2n_2}\,\cdots\,y_d^{2n_d}$$

to obtain

$$I \leq \frac{(\hbar\,\|A\|^2)^{|m|}}{2^{|j|}\,j!\,\pi^{d/2}} \sum_{|n|=|m|}\sum_{|k|=|j|} \begin{pmatrix} & |m| & \\ n_1 & \cdots & n_d \end{pmatrix} \prod_{r=1}^{d} \int y_r^{2n_r} |H_{k_r}(y_r)|^2 \exp(-y_r^2/2) dy_r.$$

Using Lemma 3.1, the one dimensional integrals in the final factor here can then be estimated as follows (without indices):

$$\int y^{2n}\,|H_k(y)|^2\,\exp(-y^2/2)\,dy$$

$$
\begin{aligned}
&\le \int_{y^2\le 2k+1} \kappa^2\, 2^k\, k!\, y^{2n}\, \exp(y^2/2)\, dy \;+\; \int 4^k\, y^{2(n+k)}\, \exp(-y^2/2)\, dy \\
&\le \kappa^2 2^k k! \frac{2}{2n+1}(2k+1)^{n+1/2}\exp(k+1/2) \;+\; 4^k 2^{(k+n+1/2)} \int z^{2(k+n)} e^{-z^2} dz \\
&= \frac{2^{k+1}}{2n+1}\kappa^2 e^{k+1/2} k! (2k+1)^{n+1/2} \;+\; 4^k 2^{(k+n+1/2)} \pi^{1/2} \frac{(2(k+n)-1)!}{2^{2(n+k)-1}(k+n-1)!} \\
&= \frac{2^{k+1}}{2n+1}\kappa^2 e^{k+1/2} k! (2k+1)^{n+1/2} \;+\; 2^{k-n+3/2} \pi^{1/2} \frac{(2(k+n)-1)!}{(k+n-1)!}. \qquad (3.12)
\end{aligned}
$$

Here we have used

$$
\int z^{2(k+n)}\, e^{-z^2}\, dz \;=\; \pi^{1/2}\, \frac{1\cdot 3\cdot 5 \cdots (2(k+n)-1)}{2^{k+n}}.
$$

Now, Stirling's formula guarantees the existence of $a > 0$, such that

$$
a^n\, n^n \le n! \le n^n, \qquad (3.13)
$$

for all integers $n \ge 1$. Using this in (3.12), we obtain

$$
\int y^{2n}\, |H_k(y)|^2\, \exp(-y^2/2)\, dy \le f_0\, f_1^{k+n}\, (k+n)!,
$$

for some constants f_0 and f_1. From this we conclude (restoring the indices)

$$
I \;\le\; \frac{(\hbar\, \|A\|^2)^{|m|}}{2^{|j|}\, j!\, \pi^{d/2}} \sum_{|n|=|m|} \sum_{|k|=|j|} f_0^d\, f_1^{|m|+|j|} \begin{pmatrix} & |m| & \\ n_1 & \cdots & n_d \end{pmatrix} (k+n)! \qquad (3.14)
$$

In this expression, we have

$$
\begin{aligned}
(k+n)! \;&=\; (|k|+|n|)! \begin{pmatrix} & |k|+|n| & \\ k_1+n_1 & \cdots & k_d+n_d \end{pmatrix}^{-1} \\
&=\; (|m|+|j|)! \begin{pmatrix} & |m|+|j| & \\ k_1+n_1 & \cdots & k_d+n_d \end{pmatrix}^{-1} \\
&\le\; (|m|+|j|)! \qquad (3.15)
\end{aligned}
$$

We further use $\sum_{|n|=|m|} \begin{pmatrix} & |m| & \\ n_1 & \cdots & n_d \end{pmatrix} = d^{|m|}$ and (2.23) in (3.14) to obtain

$$
\begin{aligned}
I \;&\le\; (\hbar\, \|A\|^2)^{|m|} \left(\frac{f_0}{\sqrt{\pi}}\right)^d (f_1\, d)^{|m|} \left(\frac{\mathrm{e}^d\, f_1}{2}\right)^{|j|} \frac{(|m|+|j|)!}{j!} \\
&=\; (\hbar\, \|A\|^2)^{|m|} \left(\frac{f_0}{\sqrt{\pi}}\right)^d (f_1\, d)^{|m|} \left(\frac{\mathrm{e}^d\, f_1}{2}\right)^{|j|} \begin{pmatrix} & |j| & \\ j_1 & \cdots & j_d \end{pmatrix} \begin{pmatrix} |m|+|j| \\ |j| \end{pmatrix} |m|! \\
&\le\; (\hbar\, \|A\|^2)^{|m|} \left(\frac{f_0}{\sqrt{\pi}}\right)^d (2\, f_1\, d)^{|m|}\, (\mathrm{e}^d\, f_1)^{|j|} \begin{pmatrix} & |j| & \\ j_1 & \cdots & j_d \end{pmatrix} |m|! \\
&\equiv (\hbar\, \|A\|^2 d)^{|m|}\, f_2^d\, f_3^{|m|}\, f_4^{|j|} \begin{pmatrix} & |j| & \\ j_1 & \cdots & j_d \end{pmatrix} |m|!, \qquad (3.16)
\end{aligned}
$$

where f_2, f_3, f_4 are numerical constants.

Estimates (3.2) and (3.16) imply

$$\left\| \frac{D^m V(\zeta(x,a))}{m!} \, (x-a)^m \, \varphi_j(A,\, B,\, \hbar,\, a,\, \eta,\, x) \right\|$$
$$\leq \; M \exp(4\tau(\delta^2 d + a^2))(\hbar \|A\|^2 (d/\delta^2) f_3)^{|m|/2} f_2^{d/2} f_4^{|j|/2} \sqrt{|m|!} \sqrt{\begin{pmatrix} & |j| & \\ j_1 & \cdots & j_d \end{pmatrix}}.$$

So, by the Schwarz inequality, (1.4), (3.9), and (3.18),

$$\left\| \frac{D^m V(\zeta(x,a))}{m!} \, (x-a)^m \, \psi_l(x,t,\hbar) \right\|^2$$
$$\leq \; \sum_{n=0}^{\widetilde{J}(l)} \sum_{|j|=n} \left\| \frac{D^m V(\zeta(x,a))}{m!} \, (x-a)^m \, \varphi_j(A,\, B,\, \hbar,\, a,\, \eta,\, x) \right\|^2$$
$$\leq \; M^2 \exp(8\tau(\delta^2 d + a^2))(\hbar \|A\|^2 (d/\delta^2) f_3)^{|m|} f_2^d |m|! \sum_{n=0}^{\widetilde{J}(l)} \sum_{|j|=n} f_4^{|j|} \begin{pmatrix} & |j| & \\ j_1 & \cdots & j_d \end{pmatrix}$$
$$= \; M^2 \, \exp(8\tau(\delta^2 d + a^2)) \, (\hbar \|A\|^2 (d/\delta^2) f_3)^{|m|} \, f_2^d \, |m|! \sum_{n=0}^{\widetilde{J}(l)} f_4^n \, d^n$$
$$= \; M^2 \, \exp(8\tau(\delta^2 d + a^2)) \, (\hbar \|A\|^2 (d/\delta^2) f_3)^{|m|} \, f_2^d \, |m|! \left(\frac{(f_4 d)^{\widetilde{J}(l)+1} - 1}{f_4 d - 1} \right)$$
$$\leq \; M^2 \, \exp(8\tau(\delta^2 d + a^2)) \, (\hbar \|A\|^2 (d/\delta^2) f_3)^{|m|} \, f_2^d \, |m|! \, 2 \, (f_4 d)^{\widetilde{J}(l)}. \tag{3.17}$$

The last step depends on the following fact: We can assume without loss that $q = f_4 d \geq 2$, so that for any positive integer p, we have $-1 \leq q^{p+1} - 2q^p$, and hence, $q^{p+1} - 1 \leq 2q^{p+1} - 2q^p$. Thus,

$$(q^{p+1} - 1)/(q-1) \leq 2q^p. \tag{3.18}$$

We use the hypothesis $|m| = l + 2$ and note that $|m|! \leq (l+2)^{l+2}$. We then conclude that there exist constants g_0 and g_1, that depend only on d and J, such that (2.13) holds. This implies the lemma. ■

4 Proofs of Lemmas 2.3 and 2.4

The proof of Lemma 2.3 relies on two preliminary lemmas.

Lemma 4.1 *The matrix elements of* $(x-a)^m$ *satisfy*

$$|\, \langle \, \varphi_j(A,\, B,\, \hbar,\, a,\, \eta,\, x),\, (x-a)^m \, \varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, x) \rangle \,|$$
$$\leq \; \hbar^{|m|/2} \, (\sqrt{2} d)^{|m|} \, \|A\|^{|m|} \, \sqrt{(|k|+1)(|k|+2) \cdots (|k|+|m|)}, \tag{4.1}$$

and

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

Proof: For $i=1,2,\cdots,d$, we can use equation (3.28) of [7] to express (x_i-a_i) in terms of raising and lowering operators. Doing so, we obtain

$$\begin{aligned}(x_i-a_i)\,\varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, x) \;&=\; \sqrt{\hbar/2}\,\sum_{p=1}^{d}\, A_{ip}\,\sqrt{k_p+1}\,\varphi_{k'(p)}(A,\, B,\, \hbar,\, a,\, \eta,\, x)\\ &\quad+\sqrt{\hbar/2}\,\sum_{p=1}^{d}\, \bar{A}_{ip}\,\sqrt{k_p}\,\varphi_{k''(p)}(A,\, B,\, \hbar,\, a,\, \eta,\, x),\end{aligned}$$

where $k'(p)$ and $k''(p)$ are constructed from k by replacing the component k_p by k_p+1 and k_p-1, respectively. Thus, $(x_i-a_i)\,\varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, x)$ may be written as a sum of $2d$ terms, each of which has the form $b_q\,\varphi_q(A,\, B,\, \hbar,\, a,\, \eta,\, x)$, where $|q|\;\le\;|k|+1$ and $|b_q|\;\le\;\sqrt{\hbar/2}\,\|A\|\,\sqrt{|k|+1}$.

From this and a simple induction, $(x-a)^m\,\varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, x)$ may be written as a sum of $(2d)^{|m|}$ terms, each of which has the form $b_q\,\varphi_q(A,\, B,\, \hbar,\, a,\, \eta,\, x)$, where $|k|-|m|\;\le\;|q|\;\le\;|k|+|m|$ and $|b_q|\;\le\;(\hbar/2)^{|m|}\,\|A\|^{|m|}\,\sqrt{(|k|+1)(|k|+2)\cdots(|k|+|m|)}$.

This implies the lemma. ∎

In the next lemma we use the shorthand $X^m(t)$ to denote $X^m(l,\, t,\, \hbar)$ of Lemma 2.3.

Lemma 4.2 *For each $N>0$, there exists $D(N)<\infty$, such that*

$$\begin{aligned}&\sup_{\{j,k:\;|j|,\,|k|\le\widetilde{J}(l)\}}\;|\,(X^{m_1}(t_1)\,X^{m_2}(t_2)\;\cdots\;X^{m_q}(t_q))_{j\,k}\,|\\ &\le\;\left(D(N)\,\sqrt{\hbar}\sup_{t\in\{t_1,t_2,\cdots t_q\}}\|A(t)\|\right)^{|m_1|+|m_2|\cdots+|m_q|}\;\widetilde{J}(l)^{(|m_1|+|m_2|+\cdots+|m_q|)/2},\end{aligned}\tag{4.2}$$

for any collection $m_1,\, m_2,\, \ldots,\, m_q$ of multi-indices that satisfy $|m_j|/\widetilde{J}(l)\le N$.

Proof: The matrix X^m is obtained from $\widetilde{X^m}$ by restricting its indices to $|j|,\,|k|\;\le\;\widetilde{J}(l)$. Using Lemma 4.1, we see that for such values of the indices,

$$\Big|\,X^m_{j\,k}(t)\,\Big|\le(\sqrt{2\hbar}\,d\,\|A(t)\|)^{|m|}\;\widetilde{J}(l)^{|m|/2}\,\sqrt{(1+1/\widetilde{J}(l))(1+2/\widetilde{J}(l)))\cdots(1+|m|/\widetilde{J}(l))}.$$

Thus, $|m|/\widetilde{J}(l)\le N$ implies

$$\Big|\,X^m_{j\,k}(t)\,\Big|\;\le\;(\sqrt{2\hbar}\,d\,\|A(t)\|)^{|m|}\,(1+N)^{|m|/2}\,\widetilde{J}(l)^{|m|/2}.$$

We estimate the absolute value of the $j,\,k$ matrix element of the product

$$\begin{aligned}&|\,(X^{m_1}(t_1)\,X^{m_2}(t_2)\;\cdots\;X^{m_q}(t_q))_{j\,k}\,|\\ &\le\;\sum_{\substack{|p_i|\,\le\,\widetilde{J}(l),\;i=1,\cdots,q-1\\ |p_1-j|\le|m_1|,|p_2-p_1|\le|m_2|,\cdots,|k-p_{q-1}|\le|m_q|}}\Big|\,X^{m_1}_{j\,p_1}(t_1)\,X^{m_2}_{p_1\,p_2}(t_2)\;\cdots\;X^{m_q}_{p_{q-1}\,k}(t_q)\,\Big|\end{aligned}\tag{4.3}$$

by bounding the absolute values of each of the matrix elements $X^{m_i}_{p_{i-1}\,p_i}(t_i)$ by

$$\left| X^{m_i}_{p_{i-1}\,p_i}(t_i) \right| \leq (\sqrt{2\hbar}\, d\, \|A(t_i)\|)^{|m_i|}\, (1+N)^{|m_i|/2}\, \widetilde{J}(l)^{|m_i|/2}, \tag{4.4}$$

and multiplying by a bound on the number of terms.

To estimate the number of terms, we first note that for any multi-index r, the number of multi-indices indices p that satisfy $\Big| |p| - |r| \Big| \leq |m|$ is equal to the number of vectors v with integer components, such that $|\sum_{i=1}^d v_i| \leq |m|$. This is bounded by the number of vectors with integer components, such that $|v_i| \leq |m|$ for $i = 1, 2, \cdots, d$, which is $(2|m|+1)^d$.

Thus, the number of terms is bounded by

$$\begin{aligned}
& \sum_{\substack{|p_i| \leq \widetilde{J}(l),\ i=1,\cdots,q-1 \\ |p_1 - j| \leq |m_1|,\, |p_2 - p_1| \leq |m_2|, \cdots, |k - p_{q-1}| \leq |m_q|}} 1 \\
\leq\ & (2|m_1|+1)^d (2|m_2|+1)^d \cdots (2|m_q|+1)^d \\
\leq\ & (e^2)^{d(|m_1|+|m_2|+\cdots+|m_q|)}.
\end{aligned} \tag{4.5}$$

The final inequality follows because $1 + 2|m_j| \leq e^{2|m_j|}$.

We obtain the lemma by using (4.4) and (4.5) to bound (4.3). ■

Proof of Lemma 2.3 We mimic the proof of Lemma 4.2. Let $\widetilde{m} = |m_0| + |m_1| + |m_2| + \ldots + |m_q|$. By Lemmas 4.1 and 4.2,

$$\begin{aligned}
& \left(\sqrt{\hbar} \sup_{t \in \{t_0, t_1, \cdots, t_q\}} \|A(t)\| \right)^{-\widetilde{m}} \left| (\widetilde{X}^{m_0}(t_0)\, X^{m_1}(t_1)\, X^{m_2}(t_2)\, \cdots\, X^{m_q}(t_q))_{j\,k} \right| \\
=\ & \left(\sqrt{\hbar} \sup_{t \in \{t_0, t_1, \cdots, t_q\}} \|A(t)\| \right)^{-\widetilde{m}} \sum_{|r| \leq \widetilde{J}(l)} \left| \widetilde{X}^{m_0}_{j\,r}(t_0) \right| \, |(X^{m_1}(t_1)\, X^{m_2}(t_2)\, \cdots\, X^{m_q}(t_q))_{r\,k}| \\
\leq\ & \sum_{\substack{r \leq \widetilde{J}(l) \\ |j-r| \leq |m_0|}} 2^{|m_0|/2} \sqrt{(|j|+1)(|j|+2)\cdots(|j|+|m_0|)} \\
& \qquad \times D(N)^{|m_1|+|m_2|+\ldots+|m_q|}\, \widetilde{J}(l)^{(|m_1|+|m_2|+\ldots+|m_q|)/2} \\
\leq\ & \sum_{\substack{|r| \widetilde{J}(l) \\ |j-r| \leq |m_0|}} 2^{|m_0|/2}\, \widetilde{J}(l)^{|m_0|/2} \sqrt{(1+1/\widetilde{J}(l))(1+2/\widetilde{J}(l))\ldots(1+|m_0|/\widetilde{J}(l))} \\
& \qquad \times D(N)^{|m_1|+|m_2|+\ldots+|m_q|}\, \widetilde{J}(l)^{(|m_1|+|m_2|+\ldots+|m_q|)/2} \\
\leq\ & \sum_{\substack{|r| \leq \widetilde{J}(l) \\ |j-r| \leq |m_0|}} 2^{|m_0|/2}\, (1+N)^{|m_0|/2}\, D(N)^{|m_1|+|m_2|+\ldots+|m_q|}\, \widetilde{J}(l)^{(|m_1|+|m_2|+\ldots+|m_q|)/2} \\
\leq\ & 2^{|m_0|/2}\, (1+N)^{|m_0|/2}\, D(N)^{|m_1|+|m_2|+\ldots+|m_q|}\, \widetilde{J}(l)^{(|m_1|+|m_2|+\ldots+|m_q|)/2} \sum_{|j-r| \leq |m_0|} 1.
\end{aligned}$$

Since the sum in the last line is $(1+2|m_0|)^d \leq e^{2d|m_0|}$, we obtain the desired estimate. ■

We now turn to the proof of Lemma 2.4. Our first step is to study the combinatorial factor $F_p(n, q)$ in the one dimensional case.

Lemma 4.3 *Let m_j denote positive integers, and let*

$$G_p(n, q) = \sum_{\substack{1 \leq m_1, m_2, \cdots, m_q \leq p \\ m_1 + m_2 + \cdots + m_q = n}} 1. \tag{4.6}$$

This quantity is zero if $n < q$ or $n > qp$. Otherwise, it satisfies

$$G_p(n, q) \leq \begin{cases} \binom{n-1}{q-1} & \text{if} \quad q \leq n \leq [q(p+1)/2] \\ \binom{q(p+1)-n-1}{q-1} & \text{if} \quad [q(p+1)/2]+1 \leq n \leq qp \end{cases} \tag{4.7}$$

Proof: If $n < q$ or $n > qp$, the sum in (4.6) contains no terms, so $G_p(n, q) = 0$.

The quantity $G_p(n, q)$ is the number of ways that the number n can be decomposed as $n = m_1 + m_2 + \ldots + m_q$ with each m_j satisfying $1 \leq m_j \leq p$. We uniquely associate to each such decomposition of n, a corresponding decomposition of $n' = q(p+1) - n = m'_1 + m'_2 + \ldots + m'_q$ by setting $m'_j = p + 1 - m_j$. This association is a one-to-one correspondence, so we see that $G_p(n, q)$ satisfies the symmetry relation

$$G_p(n, q) = G_p(q(p+1) - n, q). \tag{4.8}$$

As a consequence, the second inequality in (4.7) (with $[q(p+1)/2] + 1 \leq n \leq qp$) follows from the first (with $q \leq n \leq [q(p+1)/2]$).

To prove the first inequality in (4.7) we drop the condition $m_j \leq p$ and exactly calculate the resulting function. Dropping the upper bound on the m_j, we clearly have $G_p(n, q) \leq G(n, q)$, where

$$G(n, q) = \sum_{\substack{1 \leq m_1, m_2, \cdots, m_q \\ m_1 + m_2 + \cdots + m_q = n}} 1.$$

So, the lemma will be proved once we establish

$$G(n, q) = \binom{n-1}{q-1}. \tag{4.9}$$

To prove this, we use induction. Formula (4.9) is trivial to verify for all $n \geq 1$ when $q = 1$ and for all $n \geq 2$ when $q = 2$. Assume (4.9) has been verified whenever $n \geq q - 1$, and suppose $n \geq q$. We have

$$G(n, q) = \sum_{m_1=1}^{n-q+1} G(n - m_1, q - 1) = \sum_{m_1=1}^{n-q+1} \binom{n - m_1 - 1}{q-2},$$

so the induction step will be complete once we show

$$\sum_{m_1=1}^{n-q+1} \binom{n - m_1 - 1}{q-2} = \binom{n-1}{q-1}. \tag{4.10}$$

To prove (4.10), we do an another induction on $n \geq q$. For $n = q$ we trivially have

$$\sum_{m=1}^{1} \binom{q-2}{q-2} = 1 = \binom{q-1}{q-1}.$$

Now assume (4.10) is true for some $n \geq q$. For the case of $n+1$, we have

$$\begin{aligned}
&\sum_{m=1}^{(n+1)-q+1} \binom{(n+1)-m-1}{q-2} \\
= &\sum_{m=1}^{n-q+1} \binom{n-m}{q-2} + \binom{(n+1)-\{(n+1)-q+1\}-1}{q-2} \\
= &\sum_{m=1}^{n-q+1} \binom{n-m}{q-2} + \binom{q-2}{q-2} \\
= &\sum_{m=1}^{n-q+1} \binom{n-m}{q-2} + 1 \\
= &\sum_{m'=0}^{n-q} \binom{n-m'-1}{q-2} + 1 \\
= &\binom{n-1}{q-2} + \sum_{m'=1}^{n-q+1} \binom{n-m'-1}{q-2} - \binom{q-2}{q-2} + 1 \\
= &\binom{n-1}{q-2} + \binom{n-1}{q-1} \\
= &\binom{n}{q-1}.
\end{aligned}$$

This proves (4.10) and completes the proof of the lemma. ∎

Our next step is to obtain an estimate for $G_p(n,\, q)$ that depends only on n.

Lemma 4.4 *Let $G_p(n,\, q)$ be defined by (4.6). There exists a constant C_7, such that $p \geq 1$, $q \geq 1$, and $n \geq 1$ imply*

$$G_p(n,q)) \leq (C_7)^n. \tag{4.11}$$

Proof: We note that $G_p(n,q)$ is zero unless $q \leq n \leq qp$. Furthermore, $G_p(q,q) = G_p(qp,q) = G_2(2,1) = 1$ and $G_1(n,q) = \delta_{n\,q}$. So, we need only prove existence of C_7, such that $p \geq 2$, $q \geq 1$, $(p,q) \neq (2,1)$ imply

$$\sup_{q<n<pq} \, (G_p(n,q))^{1/n} \leq C_7. \tag{4.12}$$

To prove this, we first study the case where $q < n \leq [q(p+1)/2]$. Since $q \leq n$, we have

$$q^{1/n} \;=\; \exp(\ln(q)/n) \;\leq\; \exp(\ln(n)/n) \;\leq\; \mathrm{e}^{1/\mathrm{e}}.$$

Thus, by (4.7), the condition $q < n \leq [q(p+1)/2]$, and (3.13), we have

$$\begin{aligned}(G_p(n,\,q))^{1/n} &\leq \left(\frac{(n-1)!}{(q-1)!\,(n-q)!}\right)^{1/n}\\ &\leq q^{1/n}\left(\frac{(n-1)!}{q!\,(n-q)!}\right)^{1/n}\\ &\leq \mathrm{e}^{1/\mathrm{e}}\,\frac{n}{aq^{q/n}\,(n-q)^{(n-q)/n}}.\end{aligned} \tag{4.13}$$

An explicit computation shows that

$$\frac{\partial}{\partial n}\,\frac{n}{q^{q/n}\,(n-q)^{(n-q)/n}} \;=\; \frac{n}{q^{q/n}\,(n-q)^{(n-q)/n}}\,\frac{q}{n^2}\,\left(\,\ln(q)-\ln(n-q)\,\right).$$

From this, we deduce that the right hand side of (4.13) attains its maximum at $n = 2q$. Evaluating that maximum, we obtain

$$\sup_{q<n\leq[q(p+1)/2]}(G_p(n,\,q))^{1/n} \;\leq\; \frac{2}{a}\,\mathrm{e}^{1/\mathrm{e}}. \tag{4.14}$$

For $[q(p+1)/2] < n < pq$, the number $n' = q(p+1)-n$ satisifes $q < n' \leq [q(p+1)/2]$ and $n'/n \leq 1$. Thus, by (4.8) and (4.14), we obtain

$$\begin{aligned}(G_p(n,\,q))^{1/n} &= (G_p(n',\,q))^{1/n}\\ &\leq \left(\frac{2}{a}\,\mathrm{e}^{1/\mathrm{e}}\right)^{n'/n}\\ &\leq \frac{2}{a}\,\mathrm{e}^{1/\mathrm{e}}.\end{aligned}$$

Thus,

$$\sup_{[q(p+1)/2]<n<pq}(G_p(n,q))^{1/n} \;\leq\; \frac{2}{a}\,\mathrm{e}^{1/\mathrm{e}}. \tag{4.15}$$

Inequalities (4.14) and (4.15) imply the existence of C_7 for which (4.12) holds. This implies (4.11),and the lemma is proved. ■

We now generalize Lemma 4.4 to the multi-dimensional case.

Lemma 4.5 *Let $F_p(n,\,q)$ be defined by (2.16). For all $p \geq 1$, $q \geq 1$, and $n \geq 1$, we have*

$$F_p(n,q) \;\leq\; C_7^{(n+qd)}, \tag{4.16}$$

where C_7 is the constant of Lemma 4.4.

Proof: With m_j temporarily denoting numbers instead of multi-indices, we define

$$\Gamma_p(n,\, q) = \sum_{\substack{0\,\le\, m_1,m_2,\cdots,m_q\,\le\, p\\ m_1+m_2+\cdots+m_q\,=\,n}} 1,$$

which is zero unless $0\le n\le pq$.

By defining $m'_j = m_j+1$, we see that every decomposition of n as $n = m_1+m_2+\cdots+m_q$, with $0\le m_j\le p$, corresponds uniquely to a decomposition of $n+q$ as $n+q = m'_1+m'_2+\cdots+m'_q$, with $1\le m'_j\le p+1$. Therefore, we have the identity

$$\Gamma_p(n,\, q) \;=\; G_{p+1}(n+q,\, q). \tag{4.17}$$

We now let the m_j denote multi-indices and let $m_j(k)$ denote the k^{th} component of m_j. Then, using (4.17) and Lemma 4.4, we easily obtain

$$F_p(n,\, q) \;\le\; \sum_{\substack{0\,\le\, m_j(k)\,\le\, p\\ \sum_{j=1}^q\sum_{k=1}^d m_j(k)\,=\,n}} 1 \;=\; \Gamma_p(n,\, qd) \;\le\; C_7^{(qd+n)}.$$

■

Proof of Lemma 2.4: Suppose $2\le q\le l+2$, and let $L_q(l)$ satisfy (2.17), *i.e.*,

$$L_q(l) \;\le\; \frac{C_1^q}{\hbar^q\, q!}\sum_{n=3l-2}^{q(l+1)} (C_2\,\hbar\, l)^{n/2}\, F_{l+1}(n,\, q).$$

By Lemma 4.5 and (3.13), there exist C_8 and C_9, such that

$$\begin{aligned} L_q(l) \;&\le\; \frac{(C_1\, C_7^d)^q}{(a\,\hbar\, q)^q}\sum_{n=3l-2}^{q(l+1)} (C_2\,\hbar\, l)^{n/2}\; C_7^n \\ &\le\; \frac{C_9^q}{(\hbar\, q)^q}\sum_{n=3l-2}^{q(l+1)} \left(C_8\,\hbar^{1/2}\, l^{1/2}\right)^n. \end{aligned} \tag{4.18}$$

Note that we can take

$$C_8 \;=\; \max\{\, 1,\, \sqrt{C_2}\, C_7\,\}, \tag{4.19}$$

$$C_9 \;=\; \max\{\, 1,\, C_1\, C_7^d\,\}, \tag{4.20}$$

because we can assume $C_8\ge 1$ and $C_9\ge 1$ without loss of generality.

We arbitrarily choose two positive numbers $\alpha<1$ and $\beta<1$. We then define

$$g \;=\; \frac{1}{C_8^2}\,\min\left\{\alpha^2,\, \frac{\beta^2}{C_9^2\, C_8^4\, \mathrm{e}^{2/\mathrm{e}}}\right\}. \tag{4.21}$$

We henceforth assume $l = l(\hbar)$ is chosen to satisfy (2.18) with this value of g. With this choice, we have

$$C_8\,\hbar^{1/2}\, l^{1/2} \;\le\; \alpha. \tag{4.22}$$

By summing a geometric series in (4.18), we see that

$$L_q(l) \;\le\; \frac{C_9^q}{(1-\alpha)\,(\hbar\, q)^q}\;\left(C_8\,\hbar^{1/2}\,l^{1/2}\right)^{3l-2}$$
$$=\;\frac{C_9^q\,C_8^{2q}}{(1-\alpha)\,(\hbar\, q\, C_8^2)^q}\;\left(C_8\,\hbar^{1/2}\,l^{1/2}\right)^{3l-2}. \tag{4.23}$$

As a function of q,

$$\left(\frac{l}{q}\right)^q = \exp\left(\,q\;\ln(l/q)\,\right)$$

is maximized at $q = l/\mathrm{e}$, where it has the value $\mathrm{e}^{l/\mathrm{e}}$. Thus,

$$\left(\frac{l}{q}\right)^q \;\le\; \mathrm{e}^{l/\mathrm{e}}.$$

This, $q \le l+2$, and $\hbar\, l\, C_8^2 \;\le\; \alpha^2 \;<\; 1$ imply

$$\frac{1}{(\hbar\, q\, C_8^2)^q} \;=\; \frac{1}{(\hbar\, l\, C_8^2)^q}\left(\frac{l}{q}\right)^q \;\le\; \frac{\mathrm{e}^{l/\mathrm{e}}}{(\hbar\, l\, C_8^2)^{l+2}}.$$

From this, $C_8 \ge 1$, and $C_9 \ge 1$, we conclude

$$L_q(l) \;\le\; \frac{C_9^{l+2}\,C_8^{2(l+2)}\,\mathrm{e}^{l/\mathrm{e}}}{(1-\alpha)}\;\left(C_8\,\hbar^{1/2}\,l^{1/2}\right)^{l-6}$$
$$=\;\left(\mathrm{e}^{1/\mathrm{e}}\,C_9\,C_8^3\,\hbar^{1/2}\,l^{1/2}\right)^l\;\frac{C_9^2}{(1-\alpha)\,(\hbar\, l)^3\,C_8^2}. \tag{4.24}$$

By (4.21), we have

$$\mathrm{e}^{1/e}\,C_9\,C_8^3\,\hbar^{1/2}\,l^{1/2} \;\le\; \beta \;<\; 1.$$

Since

$$\frac{g}{\hbar} - 1 \;\le\; l \;\le\; \frac{g}{\hbar},$$

we see from (4.24) that if $\hbar \le g/2$, then we have

$$L_q(l) \;\le\; \mathrm{e}^{-|\ln(\beta)|l}\;\frac{C_9^2}{(1-\alpha)\,(g-\hbar)^3\,C_8^2}$$
$$\le\; \frac{2^3\,\mathrm{e}\,C_9^2}{(1-\alpha)\,g^3\,C_8^2}\;\mathrm{e}^{-|\ln(\beta)\,|g/\hbar}. \tag{4.25}$$

Note that the factor 2^3 can be replaced by $(1+\epsilon)$, with ϵ arbitrarily small, by taking $\hbar$ sufficiently small. ■

Remark We can choose α and β to satisfy $\frac{\beta}{\mathrm{e}^{1/\mathrm{e}}} \leq \alpha < \frac{1}{\mathrm{e}^{1/\mathrm{e}}}$. Then, since $\frac{\beta^2}{C_9^2\, C_8^4\, e^{2/e}} \leq \frac{\beta^2}{\mathrm{e}^{2/\mathrm{e}}} \leq \alpha^2$, we obtain the conclusion of Lemma 2.4 with

$$
\begin{aligned}
g &= \frac{\beta^2}{C_9^2\, C_8^6\, \mathrm{e}^{2/\mathrm{e}}}, && (4.26)\\
\gamma_1 &= \frac{|\ln(\beta)|\, \beta^2}{C_9^2\, C_8^6\, e^{2/e}} && (4.27)\\
C_3 &= \frac{2^3\, \mathrm{e}^{1+6/\mathrm{e}}\, C_9^8\, C_8^{10}}{(1-\mathrm{e}^{-1/\mathrm{e}})\, \beta^6}, && (4.28)
\end{aligned}
$$

where C_8 and C_9 are related to C_1, C_2, and C_7 by (4.19) and (4.20). Note that C_7 is purely combinatorial and has no time dependence.

5 Proof of Theorem 1.2

To prove Theorem 1.2, we revisit the proof of Theorem 1.1 and make the T dependence of all constants explicit. We then allow T to grow with $\hbar$ with the restriction that our approximation remain close to the actual solution as $\hbar \to 0$.

Lemmas 4.3, 4.4, and 4.5 have no time dependence, and the time dependence of Lemmas 2.1, 2.2, 2.3, 3.1, 4.1, and 4.2 has been made explicit in their conclusions.

Since V is bounded below and energy is conserved, $|a(t)|$ grows at most linearly with time. Thus, there exist $v_1 > 0$ and $v_0 > 0$, such that $v(t)$ defined by (2.33) satisifies

$$v(t) \leq v_0 \exp(v_1 t). \tag{5.1}$$

From assumption (1.13), it follows that

$$w(T) = \sup_{0 \leq |t| \leq T} \|A(t)\| \leq N \exp(\lambda T). \tag{5.2}$$

In the sequel, we denote all innessential constants that do not depend on T by the same symbol c.

Consider Lemma 2.2. For $z \in C_\delta(\zeta(x, a(t)))$, we can prove the existence of $\rho > 0$ such that

$$
\begin{aligned}
&\left\| \frac{D^m V(\zeta(x, a(t)))}{m!}\, (x - a(t))^m\, \psi_l(x,\, t,\, \hbar) \right\| \\
&\leq\ c \exp(\rho|t|) \left(c \sqrt{\hbar\, (l+2)}\, \exp(\lambda|t|) \right)^{l+2}.
\end{aligned} \tag{5.3}
$$

Indeed, with our bound on $|V(z)|$ we have

$$\frac{D^m V(\zeta(x, a(t)))}{m!} \leq c \exp(\rho|t|) \exp(c|x - a(t)|)$$

instead of (3.2). With this and the estimate $\exp(cy) \le \exp(cy^2) + \exp(c)$ for all $c > 0$ and $y > 0$, we see that the estimates in the proof of Lemma 2.2 are still valid. This yields (5.3). Consequently, the constants C_4 and C_5 appearing in (2.24) satisfy

$$\begin{aligned} C_4(T) &= c \exp(\rho T) \\ C_5(T) &= c \exp(\lambda T), \end{aligned}$$

where $\rho > 0$. By using estimates (5.1) and (5.2) in (2.34) and (2.35), we see that when we apply Lemma 2.4, the constants C_1 and C_2 satisfy

$$\begin{aligned} C_1(T) &= c \exp(\rho T) \\ C_2(T) &= c \exp(\lambda T). \end{aligned}$$

We still must determine the T dependence of C and γ of Theorem 1.1. We do this by determining the T dependence of g, γ_1 and C_3 in Lemma 2.4. Equations (4.19) and (4.20) yield C_8 and C_9, in terms of which the above constants are determined. We find that

$$\begin{aligned} C_8(T) &= c \exp(\lambda T/2) \\ C_9(T) &= c \exp(\rho T). \end{aligned}$$

Consequently, from (4.26), (4.27) ,(4.28), we have

$$\begin{aligned} g(T) &= c \exp(-\nu T), && \nu = 2\rho + 3\lambda \\ \gamma_1(T) &= c \exp(-\nu T), && \\ C_3(T) &= c \exp(\mu T), && \mu = 8\rho + 5\lambda. \end{aligned}$$

To arrive at these conclusions, we imposed various conditions. Those conditions were

(3.5), that now requires $\hbar \le c\exp(-2\lambda T)$,
(2.36), than now requires $c\exp(2\lambda T)\exp(-\nu T) < 1$, and
$\hbar \le g(T)/2$ used in (4.25), that now requires $\hbar \le c\exp(-\nu T)$.

These are all satisfied, provided we take

$$T(\hbar) \le T' \,|\ln(\hbar)|,$$

with $T' > 0$ sufficiently small. Using this in our estimate for the error term $\xi(t,\hbar)$, we see that for sufficiently small T', $|t| \le T' \,|\ln(\hbar)|$ implies

$$\|\psi(x,t,\hbar) - \Psi(x,t,\hbar)\|_{L^2(\mathbb{R}^d)} \le C' \exp(-\gamma'/\hbar^{\sigma}),$$

for some $\gamma' > 0$, $\sigma > 0$, and $C' > 0$. ■

References

[1] Abromowitz, M. and Stegun, I. A.: *Handbook of Mathematical Functions.* New York: Dover 1968

[2] Bambusi, D., Graffi, S., and Paul, T.: Long Time Semiclassical Approximation of Quantum Flows: A Proof of Ehrenfest Time. (1998 preprint).

[3] Combescure, M. and Robert, D.: Semiclassical Spreading of Quantum Wave Packets and Applications near Unstable Fixed Points of the Classical Flow. *Asymptotic Anal.* **14**, 377–404, (1997).

[4] Gradsteyhn, I. S. and Ryzhik, I. M.: Table of Integrals, Series, and Products, Fifth Ed. New York: Academic Press 19xx.

[5] Hagedorn, G. A.: Semiclassical Quantum Mechanics III: The Large Order Asymptotics and More General States. *Ann. Phys.* **135**, 58–70 (1981).

[6] Hagedorn, G. A.: Semiclassical Quantum Mechanics IV: Large Order Asymptotics and More General States in More than One Dimension. *Ann. Inst. H. Poincaré Sect. A.* **42**, 363–374 (1985).

[7] Hagedorn, G. A.: Raising and Lowering Operators for Semiclassical Wave Packets. *Ann. Phys.* **269**, 77–104 (1998).

[8] Jung, K.: Adiabatic Invariance and the Regularity of Perturbations. *Nonlinearity* **8**, 891-900, (1995).

[9] Robert, D.: Semi-Classical Approximation in Quantum Mechanics. A Survey of Old and Recent Mathematical Results. preprint 97/03-6, Université de Nantes, 1997.

[10] Sjöstrand, J.: *Singularités analytiques microlocales*, *Astérisque* **95**, 1982

[11] Yajima, K.: Gevrey Frequency Set and Semi-classical Behavior of Wave Packets, in *Schrödinger Operators, The Quantum Mechanical Many Body Problem*, Lecture Notes in Physics, 403, ed. by E. Balslev. Berlin, Heidelberg, New York: Springer-Verlag, 1992, pp 248–264.