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Semiclassical Quantum Mechanics

I. The $\hbar \to 0$ Limit for Coherent States

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Abstract. We consider the $\hbar \to 0$ limit of the quantum dynamics generated by the Hamiltonian $H(\hbar) = -(\hbar^2/2m)\Delta + V$. We prove that the evolution of certain Gaussian states is determined asymptotically as $\hbar \to 0$ by classical mechanics. For suitable potentials V in $n \geqq 3$ dimensions, our estimates are uniform in time and our results hold for scattering theory.

1. Introduction and Results

The purpose of this paper is to give simple proofs of two theorems concerning the classical limit of quantum mechanics. Our first theorem deals with finite times. The second deals with infinite times in the framework of scattering theory.

For the potentials which we consider, the quantum Hamiltonian $H(\hbar) = -(\hbar^2/2m)\Delta + V(x) = H_0(\hbar) + V$ on $L^2(\mathbb{R}^n)$ is essentially self-adjoint on the $C^\infty(\mathbb{R}^n)$ functions of compact support. The corresponding classical Hamiltonian is $H(\xi, x) = \xi^2/2m + V(x)$ on the phase space $\mathbb{R}^{2n}$.

Under the Hamiltonian $H(\hbar)$ we study the evolution of the Gaussian wave functions $\psi_\alpha(A, B, \hbar, a, \eta, x)$ which are defined below. The state $\psi_\alpha(A, B, \hbar, a, \eta, x)$ is concentrated near the position a and near the momentum η. Heuristically, its position width and momentum width are given by the matrices $\hbar^\alpha(AA^*)^{1/2}$ and $(\hbar^{1-\alpha}/2)(BB^*)^{1/2}$, respectively. Our motivation for considering the states $\psi_\alpha(A, B, \hbar, a, \eta, x)$ comes from explicit calculations for harmonic oscillators. The precise definition is the following:

Definition. Let A and B be complex $n \times n$ matrices with the following properties:

A and B are invertible; (1.1)

BA^{-1} is symmetric ((real symmetric) + i (real symmetric)); (1.2)

$\mathrm{Re}\, BA^{-1} = \frac{1}{2}[(BA^{-1}) + (BA^{-1})^*]$ is strictly positive definite; (1.3)

$(\mathrm{Re}\, BA^{-1})^{-1} = AA^*$. (1.4)

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For $a \in \mathbb{R}^n$, $\eta \in \mathbb{R}^n$, $\alpha \in \mathbb{R}$, and $\hbar > 0$, we define

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

The choice of the square root in this definition will depend on the context and will always be specified.

Remarks. 1. If A and B satisfy conditions (1.1)–(1.4), then these conditions are also satisfied when A and B are interchanged, i.e., $(\mathrm{Re}\, AB^{-1})^{-1} = BB^*$. See the proof of Lemma 2.1.

2. Whenever we write $\psi_\alpha(A, B, \hbar, a, \eta, x)$, we tacitly assume that conditions (1.1)–(1.4) are fulfilled.

3. If A and B satisfy conditions (1.1)–(1.4), then $\|\psi_\alpha(A, B, \hbar, a, \eta, \cdot)\| = 1$.

4. Any normalized Gaussian has the form $\psi_\alpha(A, B, \hbar, a, \eta, x)$ for some choice of A, B, $\hbar$, a, and η. To see this we note that the quadratic form in any Gaussian is given by an invertible symmetric matrix Q, whose real part $\frac{1}{2}(Q + Q^*) = \frac{1}{2}(Q + \bar{Q})$ is strictly positive definite. We can choose $\hbar = 1$, $A = (\mathrm{Re}\, Q)^{-1/2}$, and $B = QA$. The a and η are unique and easy to find.

5. The matrices A and B are not unique. Nothing is changed if we multiply both A and B on the right by the same unitary matrix whose determinant is 1.

6. For each $\hbar > 0$ we define the Fourier Transform, $\mathcal{F}_\hbar$, by

$$[\mathcal{F}_\hbar \psi](\xi) = (2\pi\hbar)^{-n/2} \int_{\mathbb{R}^n} e^{-i\langle \xi, x\rangle/\hbar} \psi(x) dx.$$

The inverse transform, $\mathcal{F}_\hbar^{-1}$, is given by

$$[\mathcal{F}_\hbar^{-1} \phi](x) = (2\pi\hbar)^{-n/2} \int_{\mathbb{R}^n} e^{i\langle x, \xi\rangle/\hbar} \phi(\xi) d\xi.$$

We denote $[\mathcal{F}_\hbar \psi_\alpha(A, B, \hbar, a, \eta, \cdot)](\xi)$ by $\hat{\psi}_\alpha(A, B, \hbar, a, \eta, \xi)$. Explicitly,

$$\begin{aligned}\hat{\psi}_\alpha&(A, B, \hbar, a, \eta, \xi)\\ &= (\pi/2)^{-n/4} \hbar^{-n(1-\alpha)/2} (\det B)^{-1/2} \exp\{-\hbar^{2\alpha-2} \langle (\xi - \eta), AB^{-1}(\xi - \eta)\rangle \\ &\quad - i\langle a, \xi\rangle/\hbar\}\\ &= \psi_{1-\alpha}(B/2, 2A, \hbar, \eta, -\alpha, \xi) e^{-i\langle \eta, a\rangle/\hbar}.\end{aligned}$$

We must be careful about the branch of the square root. The choice of the branch is independent of a, η, and ξ, so we take them all to be zero. Next, we notice that

$$\begin{aligned}\int_{\mathbb{R}^n} &(2\pi)^{-n/4} \hbar^{-n\alpha/2} \exp\{-(4\hbar^{2\alpha})^{-1} \langle x, [\mathrm{Re}\, BA^{-1} + iz\, \mathrm{Im}\, BA^{-1}]\, x\rangle\}\, dx\\ &= (\pi/2)^{-n/4} \hbar^{-n(1-\alpha)/2} (\det[\mathrm{Re}\, BA^{-1} + iz\, \mathrm{Im}\, BA^{-1}])^{-1/2}\end{aligned}$$

must be positive when $z = 0$. Furthermore, this integral is analytic for z in some complex neighborhood of the real interval $[0, 1]$. This determines $(\det BA^{-1})^{1/2}$, which determines the branch of $(\det B)^{-1/2} = (\det BA^{-1})^{-1/2} (\det A)^{-1/2}$ from the choice of $(\det A)^{-1/2}$.

The following notation will be used throughout the paper: For $V \in C^2(\mathbb{R}^n)$, $V^{(1)}(x)$ denotes the gradient $\left(\frac{\partial V}{\partial x_i}(x)\right)$, and $V^{(2)}(x)$ denotes the Hessian $\left(\frac{\partial^2 V}{\partial x_i\, \partial x_j}(x)\right)$.

The Euclidean norm of $V^{(1)}(x)$ is $|V^{(1)}(x)|$, and the operator norm of $V^{(2)}(x)$ on $\mathbb{R}^n$ is $\|V^{(2)}(x)\|$.

With this notation, we can now state our first theorem.

Theorem 1.1. *Suppose* $1/3<\alpha<2/3$, $V\in C^2(\mathbb{R}^n)$, $|V(x)|\leqq C_1 e^{Mx^2}$, *and* $V\geqq -C_2$. *Assume* $V^{(2)}$ *is uniformly Lipschitz on compact subsets of* $\mathbb{R}^n$ *(i.e., given any* $R>0$, *there exists* β, *such that* $\|V^{(2)}(x)-V^{(2)}(y)\|\leqq\beta|x-y|$ *whenever* $|x|<R$ *and* $|y|<R$*). Let* $a_0\in\mathbb{R}^n$, $\eta_0\in\mathbb{R}^n$, *and let* A_0 *and* B_0 *satisfy conditions* (1.1)–(1.4). *Then for each* $T>0$ *and each positive* $\lambda<\operatorname{Min}\{3\alpha-1,2-3\alpha\}$, *there exist* C *and* $\delta>0$ *such that* $\hbar<\delta$ *implies*

$$\begin{aligned}&\|e^{-itH(\hbar)/\hbar}\psi_\alpha(A_0,B_0,\hbar,a_0,\eta_0,\cdot)\\ &\quad -e^{iS(t)/\hbar}\psi_\alpha(A(t),B(t),\hbar,a(t),\eta(t),\cdot)\|\leqq C\hbar^\lambda,\end{aligned}\tag{1.5}$$

whenever $|t|\leqq T$ *(*$\det A(t)$ *is never zero, and the branch of the square root* $(\det A(t))^{-1/2}$ *in the definition of* $\psi_\alpha(A(t), B(t), \hbar, a(t), \eta(t), x)$ *is determined by continuity in* t*). Here* $[A(t), B(t), a(t), \eta(t), S(t)]$ *is the unique solution to the system of coupled ordinary differential equations:*

$$\frac{d\eta}{dt}(t)=-V^{(1)}(a(t)),\tag{1.6}$$

$$\frac{da}{dt}(t)=\eta(t)/m,\tag{1.7}$$

$$\frac{dA}{dt}(t)=i\hbar^{1-2\alpha}B(t)/2m,\tag{1.8}$$

$$\frac{dB}{dt}(t)=2i\hbar^{2\alpha-1}V^{(2)}(a(t))A(t),\tag{1.9}$$

$$\frac{dS}{dt}(t)=(\eta(t))^2/2m-V(a(t)),\tag{1.10}$$

subject to the conditions $A(0)=A_0$, $B(0)=B_0$, $a(0)=a_0$, $\eta(0)=\eta_0$, *and* $S(0)=0$.

Furthermore, the differentials $\dfrac{\partial a(t)}{\partial a(0)}$, $\dfrac{\partial a(t)}{\partial\eta(0)}$, $\dfrac{\partial\eta(t)}{\partial a(0)}$, *and* $\dfrac{\partial\eta(t)}{\partial\eta(0)}$ *exist, and*

$$A(t)=\frac{\partial a(t)}{\partial a(0)}A(0)+\tfrac{1}{2}i\hbar^{1-2\alpha}\frac{\partial a(t)}{\partial\eta(0)}B(0),\tag{1.11}$$

$$B(t)=\frac{\partial\eta(t)}{\partial\eta(0)}B(0)-2i\hbar^{2\alpha-1}\frac{\partial\eta(t)}{\partial a(0)}A(0).\tag{1.12}$$

Remarks. 1. In the above theorem $a(t)$ and $\eta(t)$ are, of course, the classical position and momentum at time t. $S(t)$ is the classical action.

2. Equations (1.11) and (1.12) show that the spreading is also determined asymptotically as $\hbar\to 0$ by classical mechanics. The classical paths which are "near" the path $(a(t),\eta(t))$ determine the spreading in time. Of course, the meaning of "near" depends on $\hbar^\alpha A_0$ and $\hbar^{1-\alpha}B_0$. For example, if $\alpha<1/2$, then as $\hbar\to 0$, $A(t)$ is asymptotic to $\dfrac{\partial a(t)}{\partial a(0)}A(0)$. In this case the behavior of $A(t)$ as $\hbar\to 0$ is determined by

the paths which have initial positions approximately equal to $a(0)$ and have initial momenta *equal* to $\eta(0)$. If $\alpha > 1/2$, then the asymptotic behavior of $A(t)$ as $\hbar \to 0$ is determined by the paths which have initial positions *equal* to $a(0)$ and initial momenta approximately equal to $\eta(0)$. The same results hold for $B(t)$.

3. The branch of the square root $(\det A(t))^{-1/2}$ is related to the Maslov index of the path $(a(t), \eta(t))$ [1, 3, 10]. So, from our point of view, the Maslov index is simply a winding number. The position space caustics (which are usually mentioned in connection with the index) are the points at which $\left(\det \frac{\partial a(t)}{\partial a(0)}\right) = 0$ or $\left(\det \frac{\partial a(t)}{\partial \eta(0)}\right) = 0$. As mentioned above, when $\alpha < 1/2$, $A(t)$ is asymptotic to $\frac{\partial a(t)}{\partial a(0)} A(0)$. Since $\hbar^{n\alpha} |\det A(t)|$ is essentially the volume of the set on which $|\psi_\alpha(A(t), B(t), \hbar, a(t), \eta(t), x)|$ is large, we see that our wave function is exceptionally singular at those times when $\left(\det \frac{\partial a(t)}{\partial a(0)}\right) = 0$ as $\hbar \to 0$.

The momentum space caustics are the points at which $\left(\det \frac{\partial \eta(t)}{\partial \eta(0)}\right) = 0$ or $\left(\det \frac{\partial \eta(t)}{\partial a(0)}\right) = 0$. These give rise to singular behavior of $\hat{\psi}_\alpha(A(t), B(t), \hbar, a(t), \eta(t), \xi)$ as $\hbar \to 0$.

4. Our proof of Theorem 1.1 involves little more than the Trotter product formula [11] and the approximation of V by its second order Taylor expansion. For harmonic oscillators, our approximate evolution is consequently exact!

5. Classical particles can be "captured" if they have just enough energy to get to the top of a potential hill (see [14, Appendix 2]). Such capture processes contribute to exceptional sets in classical scattering. There are no such exceptional sets in quantum scattering, and it is instructive to see what happens to a semiclassical particle in one dimension. At the top of the hill, $V^{(2)}(x)$ is negative. So, Eqs. (1.8) and (1.9) show that the position width function $\hbar^\alpha A(t)$ is approximately a linear combination of exponentials. Generically, such a linear combination diverges exponentially in time. The behavior of the momentum width function $\hbar^{1-\alpha} B(t)$ is similar.

6. Theorem 1.1 is related to a theorem of Hepp [7] which is concerned with expectation values of Weyl operators in coherent states as $\hbar \to 0$. Yajima's papers [15, 16] implicitly contain Theorem 1.1, although Yajima focuses his attention on infinite time problems.

Our second theorem deals with scattering theory. For potentials $V \in L^\infty(\mathbb{R}^n)$ which satisfy $|V(x)| \leq c(1+|x|)^{-1-\varepsilon}$, the quantum mechanical wave operators

$$\Omega^\pm(\hbar) = \underset{t \to \mp\infty}{\text{strong-lim}}\, e^{itH(\hbar)/\hbar} e^{-itH_0(\hbar)/\hbar}$$

exist for each $\hbar > 0$. Furthermore, they are asymptotically complete: $\mathrm{Ran}(\Omega^+(\hbar)) = \mathrm{Ran}(\Omega^-(\hbar)) =$ the continuous subspace for $H(\hbar)$ (see e.g., [4.12]). This implies the unitarity of the quantum S-matrix, $\mathbf{S}(\hbar) = \Omega^-(\hbar)^* \Omega^+(\hbar)$.

If a potential $V \in C^3(\mathbb{R}^n)$ satisfies $\|V^{(j)}(x)\| \leqq c_j(1+|x|)^{-1-j-\nu}$ for $0 \leqq j \leqq 3$ and some $\nu > 0$, then given any $a_- \in \mathbb{R}^n$ and $\eta_- \in \mathbb{R}^n$ with $\eta_- \neq 0$, there exists a unique solution $[a(t), \eta(t)]$ to Eqs. (1.6)–(1.7), such that

$$\lim_{t \to -\infty} |a(t) - a_- - \eta_- t/m| = 0 \tag{1.13}$$

and

$$\lim_{t \to -\infty} |\eta(t) - \eta_-| = 0 . \tag{1.14}$$

Furthermore, there is a closed set $\mathscr{E} \subseteq \{(a_-, \eta_-) \in \mathbb{R}^{2n} : \eta_- \neq 0\}$ of Lebesgue measure zero in $\mathbb{R}^{2n}$, such that $(a_-, \eta_-) \notin \mathscr{E}$ implies the existence of a_+ and $\eta_+ \neq 0$ such that

$$\lim_{t \to +\infty} |a(t) - a_+ - \eta_+ t/m| = 0 \tag{1.15}$$

and

$$\lim_{t \to +\infty} |\eta(t) - \eta_+| = 0 . \tag{1.16}$$

For proofs of these facts, see [8, 12, 13, 14]. The classical S-matrix, $\mathbf{S}_{c\ell} : \mathbb{R}^{2n} \backslash \mathscr{E} \to \mathbb{R}^{2n}$ is defined by $\mathbf{S}_{c\ell}(a_-, \eta_-) = (a_+, \eta_+)$.

Theorem 1.2. *Let $n \geqq 3$ and $\alpha \in (1/3, 2/3)$. For some $\nu > 0$, assume $V \in C^3(\mathbb{R}^n)$ satisfies*

$$\|V^{(j)}(x)\| \leqq c_j(1+|x|)^{-1-j-\nu} \quad \text{for} \quad 0 \leqq j \leqq 3 .$$

Suppose $(a_-, \eta_-) \in \mathbb{R}^{2n} \backslash \mathscr{E}$, and suppose A_- and B_- are complex $n \times n$ matrices satisfying conditions (1.1)–(1.4). Then there exist $\eta_+ \neq 0$, $a_+ \in \mathbb{R}^n$, $S_+ \in \mathbb{R}$, matrices A_+ and B_+ satisfying conditions (1.1)–(1.4), and a unique solution $[A(t), B(t), a(t), \eta(t), S(t)]$ to the system (1.6)–(1.10), such that Eqs. (1.13)–(1.16) hold, and the following asymptotic conditions are satisfied:

$$\lim_{t \to \pm\infty} \|A(t) - A_\pm - i\hbar^{1-2\alpha} B_\pm t/2m\| = 0 , \tag{1.17$_\pm$}$$

$$\lim_{t \to \pm\infty} \|B(t) - B_\pm\| = 0 , \tag{1.18$_\pm$}$$

$$\lim_{t \to -\infty} |S(t) - t(\eta_-)^2/2m| = 0 , \tag{1.19}$$

and

$$\lim_{t \to +\infty} |S(t) - S_+ - t(\eta_+)^2/2m| = 0 . \tag{1.20}$$

The functions $a(t)$, a_+, $\eta(t)$, and η_+ are differentiable functions of a_- and η_-, and the following relations hold:

$$A(t) = \frac{\partial a(t)}{\partial a_-} A_- + \tfrac{1}{2} i\hbar^{1-2\alpha} \frac{\partial a(t)}{\partial \eta_-} B_- , \tag{1.21}$$

$$B(t) = \frac{\partial n(t)}{\partial \eta_-} B_- - 2i\hbar^{2\alpha-1} \frac{\partial \eta(t)}{\partial a_-} A_- , \tag{1.22}$$

$$A_+ = \frac{\partial a_+}{\partial a_-} A_- + \tfrac{1}{2} i\hbar^{1-2\alpha} \frac{\partial a_+}{\partial \eta_-} B_- , \tag{1.23}$$

$$B_+ = \frac{\partial \eta_+}{\partial \eta_-} B_- - 2i\hbar^{2\alpha-1} \frac{\partial \eta_+}{\partial a_-} A_- . \tag{1.24}$$

For each $\lambda < \mathrm{Min}\{3\alpha - 1, 2 - 3\alpha\}$, *there exists* C *such that* $\hbar \leqq 1$ *implies*

$$\sup_{t \in \mathbb{R}} \| e^{-itH(\hbar)/\hbar} \Omega^+(\hbar) \psi_\alpha(A_-, B_-, \hbar, a_-, \eta_-, \cdot) - e^{iS(t)/\hbar} \psi_\alpha(A(t), B(t), \hbar, a(t), \eta(t), \cdot) \| < C\hbar^\lambda, \tag{1.25}$$

and

$$\| \mathbf{S}(\hbar) \psi_\alpha(A_-, B_-, h, a_-, \eta_-, \cdot) - e^{iS_+/\hbar} \psi_\alpha(A_+, B_+, \hbar, a_+, \eta_+, \cdot) \| < C\hbar^\lambda. \tag{1.26}$$

To determine the branch of the square root, $(\det A(t))^{-1/2}$, *which occurs in Eq.* (1.25), *we first notice that* $(\det A_-)^{-1/2}$ *determines* $(\det[A_- + i\hbar^{1-2\alpha} B_- t/2m])^{-1/2}$ *by continuity from* $t = 0$. *Next,* $(\det A(t))^{-1/2}$ *is determined by continuity and the requirement*

$$\lim_{t \to -\infty} (\det A(t))^{-1/2} - (\det[A_- + i\hbar^{1-2\alpha} B_- t/2m])^{-1/2} = 0.$$

Similarly, $(\det A_+)^{-1/2}$ *in* (1.26) *is determined from* $(\det A(t))^{-1/2}$, *continuity in t, and the two requirements*

$$\lim_{t \to 0} (\det A(t))^{-1/2} - (\det(A(t) - i\hbar^{1-2\alpha} B_+ t/2m))^{-1/2} = 0,$$

and

$$\lim_{t \to \infty} (\det A_+)^{-1/2} - (\det(A(t) - i\hbar^{1-2\alpha} B_+ t/2m))^{-1/2} = 0.$$

Remarks. 1. Yajima's theorem [15] deals with the case $\alpha = 1$ with less restrictive conditions on the states which are considered. However, Yajima has not proved that his exceptional set has measure zero. See [16] for results on long range scattering.

2. Our methods can easily be generalized to handle a Coulomb singularity. Of course, the exceptional set $\mathscr{E}$ must be increased to include paths which hit the singularity, but this larger set is again a closed set of measure zero in $\mathbb{R}^{2n}$. Our method can therefore be extended to include Yukawa potentials.

3. The classical field limit of scattering which has been studied by Ginibre and Velo [5, 6] should not be confused with the limits we are studying. The problems which they are addressing are very different from ours.

2. Finite Times

In this section we prove Theorem 1.1. We begin with three preliminary lemmas. The first one deals with solutions of certain matrix valued differential equations, such as Eqs. (1.8) and (1.9). The second gives exact formulas for $e^{-itH_0(\hbar)/\hbar} \psi_\alpha(A, B, \hbar, a, \eta, x)$ and $e^{-itW/\hbar} \psi_\alpha(A, B, \hbar, a, \eta, x)$, where W is any quadratic polynomial on $\mathbb{R}^n$. The third lemma contains the crucial estimate to be used to prove Eq. (1.5). Modulo technicalities, Theorem 1.1 follows easily from these lemmas and the Trotter product formula.

Lemma 2.1. *Let* $f(t)$ *and* $g(t)$ *be real symmetric* $n \times n$ *matrix valued functions on* $[-T, T]$ *such that* $\|f(t) - f(s)\| + \|g(t) - g(s)\| \leqq \beta |t - s|$ *for some* β. *Let* A_0 *and* B_0 *be* *complex matrices which satisfy conditions* (1.1)–(1.4). *Then for* $|t| \leq T$ *there exists a unique bounded solution* $[A(t), B(t)]$ *to the equations*

$$\frac{dA}{dt}(t) = i f(t) B(t), \tag{2.1}$$

$$\frac{dB}{dt}(t) = i g(t) A(t), \tag{2.2}$$

such that $A(0) = A_0$ *and* $B(0) = B_0$. *Moreover,* $A(t)$ *and* $B(t)$ *satisfy conditions* (1.1)–(1.4).

Proof. The existence, uniqueness, and boundedness are standard results for ordinary differential equations (see e.g., [2]).

Let $F(t) = A(t)^* B(t) + B(t)^* A(t)$ and $G(t) = A(t)^t B(t) - B(t)^t A(t)$. Equations (2.1) and (2.2) and the conditions on $f(t)$ and $g(t)$ show

$$\begin{aligned} F'(t) &= A(t)^* B'(t) + A'(t)^* B(t) + B(t)^* A'(t) + B'(t)^* A(t) \\ &= iA(t)^* g(t) A(t) - iB(t)^* f(t) B(t) + iB(t)^* f(t) B(t) - iA(t)^* g(t) A(t) \\ &= 0, \end{aligned}$$

and

$$\begin{aligned} G'(t) &= A(t)^t B'(t) + A'(t)^t B(t) - B(t)^t A'(t) - B'(t)^t A(t) \\ &= iA(t)^t g(t) A(t) + iB(t)^t f(t) B(t) - iB(t)^t f(t) B(t) - iA(t)^t g(t) A(t) \\ &= 0. \end{aligned}$$

Thus, $F(t)$ and $G(t)$ are constant. Since $(\mathrm{Re}\, B_0 A_0^{-1})^{-1} = A_0 A_0^*$,

$$F(t) = F(0) = A_0^* [B_0 A_0^{-1} + (B_0 A_0^{-1})^*] A_0 = 2A_0^* (\mathrm{Re}\, B_0 A_0^{-1}) A_0 = 2I.$$

So for $z \in \mathbb{C}^n$, $2\langle z, z\rangle = \langle z, F(t) z\rangle = \langle A(t) z, B(t) z\rangle + \langle B(t) z, A(t) z\rangle$ is zero only if $z = 0$. Thus, $\ker A(t) = \ker B(t) = \{0\}$ and both $A(t)$ and $B(t)$ are invertible.

We can now easily verify relation (1.4) for $A(t)$ and $B(t)$:

$$\begin{aligned} A(t) A(t)^* &= \{\tfrac{1}{2} [A(t)^{-1}]^* F(t) A(t)^{-1}\}^{-1} \\ &= \{\tfrac{1}{2} [B(t) A(t)^{-1} + (B(t) A(t)^{-1})^*]\}^{-1} \\ &= (\mathrm{Re}\, B(t) A(t)^{-1})^{-1}. \end{aligned}$$

This relation and the invertibility of $A(t)$ ensure that $\mathrm{Re}\, B(t) A(t)^{-1}$ is strictly positive definite.

Since $B_0 A_0^{-1}$ is symmetric, $G(t) = G(0) = A_0^t [B_0 A_0^{-1} - (B_0 A_0^{-1})^t] A_0 = 0$. Thus, $0 = [A(t)^t]^{-1} G(t) A(t)^{-1} = B(t) A(t)^{-1} - [B(t) A(t)^{-1}]^t$, and $B(t) A(t)^{-1}$ is symmetric. □

Lemma 2.2. *Choose* $A, B, \hbar, a, \eta$, *and* α *as in the definition of* $\varphi_\alpha(A, B, \hbar, a, \eta, \cdot) \in L^2(\mathbb{R}^n)$.

Let $W(x) = W(a) + \langle W^{(1)}(a), (x-a)\rangle + \frac{1}{2}\langle (x-a), W^{(2)}(a)(x-a)\rangle$ *be a second order polynomial on* $\mathbb{R}^n$. *Then,*

$$\begin{aligned} & e^{-itW/\hbar} \varphi_\alpha(A, B, \hbar, a, \eta, x) \\ &\quad = e^{-itW(a)/\hbar} \varphi_\alpha(A, B + 2it\hbar^{2\alpha-1} W^{(2)}(a) A, \hbar, a, \eta - t W^{(1)}(a), x), \end{aligned}$$

and

$$e^{-itH_0(\hbar)/\hbar}\psi_\alpha(A,B,\hbar,a,\eta,x)$$
$$=e^{it\langle\eta,\eta\rangle/2m\hbar}\psi_\alpha(A+it\hbar^{1-2\alpha}B/2m,B,\hbar,a+t\eta/m,\eta,x).$$

Continuity in t determines the choice of the square roots in the definitions of the ψ_α's on the right hand sides of the above equations.

Proof. Verification of the first result is a trivial algebraic exercise. To compute $e^{-itH_0(\hbar)/\hbar}\psi_\alpha$, we exploit the fact that

$$[\mathscr{F}_\hbar e^{-itH_0(\hbar)/\hbar}\psi_\alpha(A,B,\hbar,a,\eta,\cdot)](\xi)$$
$$=e^{-it\langle\xi,\xi\rangle/2m\hbar}\hat{\psi}_\alpha(A,B,\hbar,a,\eta,\xi)$$
$$=e^{it\langle\eta,\eta\rangle/2m\hbar}\hat{\psi}_\alpha(A+it\hbar^{1-2\alpha}B/2m,\ B,\ \hbar,\ a+t\eta/m,\eta,\xi).$$

Applying the inverse Fourier transform, we see that we need only show $(\mathrm{Re}\,B(A+it\hbar^{1-2\alpha}B/2m)^{-1})^{-1}=AA^*$ and that $B(A+it\hbar^{1-2\alpha}B/2m)^{-1}$ is symmetric. This follows from Lemma 2.1 with $f(t)=\hbar^{1-2\alpha}/2m$ and $g(t)=0$. □

Lemma 2.3. *Suppose $\alpha>1/3$, $f\in L^\infty(\mathbb{R}^n)$, $V\in C^2(\mathbb{R}^n)$, $|V(x)|\leqq C_1e^{M|x|^2}$, and $V^{(2)}$ is uniformly Lipshitz on compact subsets of $\mathbb{R}^n$ (i.e. given any $R>0$, there exists β such that $\|V^{(2)}(x)-V^{(2)}(y)\|\leqq\beta|x-y|$ whenever $|x|<R$ and $|y|<R$). Let $K\subseteqq\mathbb{R}^n$ be compact. Define*

$$W_y(x)=V(y)+\langle V^{(1)}(y),(x-y)\rangle+\tfrac{1}{2}\langle(x-y),V^{(2)}(y)(x-y)\rangle.$$

Then for each $N>0$, $p<\alpha$, and $\gamma\in(0,\alpha-p)$, there exist C_2 and $\delta\in(0,1)$ such that

$$\|(e^{-isV/\hbar}-e^{-isW_y/\hbar})f\psi_\alpha(A,B,\hbar,y,\eta,\cdot)\|\leqq C_2\|f\|_\infty|s|\hbar^{3\gamma-1}$$

for all $s\in\mathbb{R}$ whenever $\|A\|\leqq N\hbar^{-p}$, $y\in K$, and $\hbar<\delta$.

Proof. The hypotheses on V imply the existence of β, such that $y\in K$ and $|x-y|\leqq 1$ imply $|V(x)-W_y(x)|\leqq\beta|x-y|^3$.

Let $X_1(\hbar,y,\cdot)$ and $X_2(\hbar,y,\cdot)$ denote the characteristic functions of $\{x:|x-y|\leqq\hbar^\gamma\}$ and $\{x:|x-y|>\hbar^\gamma\}$, respectively. Then, for $\hbar\leqq 1$,

$$\|(e^{-isV/\hbar}-e^{-isW_y/\hbar})f\psi_\alpha(A,B,\hbar,y,\eta,\cdot)\|$$
$$\leqq\|f\|_\infty\hbar^{-1}|s|\,\||V-W_y|\psi_\alpha(A,B,\hbar,y,\eta,\cdot)\|$$
$$\leqq\|f\|_\infty\hbar^{-1}|s|\,[\|X_1(\hbar,y,\cdot)|V-W_y|\psi_\alpha(A,B,\hbar,y,\eta,\cdot)\|$$
$$+\|X_2(\hbar,y,\cdot)|V-W_y|\psi_\alpha(A,B,\hbar,y,\eta,\cdot)\|]$$
$$\leqq\|f\|_\infty[\beta|s|\hbar^{3\gamma-1}+C'\hbar^{-1}|s|\,\|X_2(\hbar,y,x)e^{M|x|^2}\psi_\alpha(A,B,\hbar,y,\eta,x)\|].$$

Since $y\in K$, we now need only show $\|X_2(\hbar,y,x)e^{M|x-y|^2}\psi_\alpha(A,B,\hbar,y,\eta,x)\|$ is less than some constant multiple of $\hbar^{3\gamma}$ whenever $\hbar^p\|A\|\leqq N$ and $\hbar$ is less than some $\delta>0$. However, (1.4) shows that

$$\|X_2(\hbar,y,x)e^{M|x-y|^2}\psi_\alpha(A,B,\hbar,y,\eta,x)\|$$
$$\leqq\|X_2(\hbar,y,x)\exp\{M|x-y|^2-(8\hbar^{2\alpha})^{-1}\langle(x-y),(AA^*)^{-1}(x-y)\rangle\}\|_\infty$$
$$\cdot\|(2\pi)^{-n/4}\hbar^{-n\alpha/2}(\det A)^{-1/2}\exp\{-(8\hbar^{2\alpha})^{-1}\langle(x-y),(AA^*)^{-1}(x-y)\rangle\}\|$$
$$=2^{n/2}\exp\{M\hbar^{2\gamma}-\|A\|^{-2}\hbar^{-2\alpha+2\gamma}/8\}$$

whenever $M-\|A\|^{-2}\hbar^{-2\alpha}/8$ is negative. Since $\|A\|\leqq N\hbar^{-p}$ and $p<\alpha$, there obviously exists $\delta>0$ such that $\hbar<\delta$ implies

$$M-\|A\|^{-2}\hbar^{-2\alpha}/8\leqq M-\hbar^{-2\alpha+2p}/8N^2$$

is negative. Furthermore, since $\gamma<\alpha-p$, there exist C'' such that $\hbar<\delta$ implies $2^{n/2}\exp\{M\hbar^{2\gamma}-\hbar^{-2\alpha+2p+2\gamma}/8N^2\}\leqq C''\hbar^{3\gamma}$. This implies the lemma. □

Proof of Theorem 1.1. The hypotheses on V guarantee the existence of a unique bounded solution to the system (1.6)–(1.10) for $|t|\leqq T$ (see e.g., [2, Sect. V.11]; energy conservation shows that a and η are bounded). Furthermore, $\frac{\partial a(t)}{\partial a(0)}$, $\frac{\partial a(t)}{\partial \eta(0)}$, $\frac{\partial \eta(t)}{\partial a(0)}$, and $\frac{\partial \eta(t)}{\partial \eta(0)}$ exist [2, Sect. V.12]. Equations (1.6) and (1.7) imply

$$a(t)=a(0)+\eta(0)t/m-m^{-1}\int_0^t(t-s)V^{(1)}(a(s))ds.$$

Differentiating this with respect to $a(0)$ and $\eta(0)$, we have

$$\frac{\partial a(t)}{\partial a(0)}=I-m^{-1}\int_0^t(t-s)V^{(2)}(a(s))\frac{\partial a(s)}{\partial a(0)}ds$$

and

$$\frac{\partial a(t)}{\partial \eta(0)}=It/m-m^{-1}\int_0^t(t-s)V^{(2)}(a(s))\frac{\partial a(s)}{\partial \eta(0)}ds.$$

These are two independent solutions to the linear equation

$$\frac{d^2f}{dt^2}(t)=-m^{-1}V^{(2)}(a(t))f(t).$$

From Eqs. (1.8) and (1.9), we see that $A(t)$ also satisfies this equation. Consequently, (1.11) holds for all $t\in[-T,T]$, since the correct boundary conditions are satisfied at $t=0$.

To verify (1.12), we first notice that $\frac{d}{dt}\frac{\partial a(t)}{\partial a(0)}$ and $\frac{\partial}{\partial a(0)}\frac{da(t)}{dt}=m^{-1}\frac{\partial \eta(t)}{\partial a(0)}$ are continuous. It follows that $\frac{d}{dt}\frac{\partial a(t)}{\partial a(0)}=m^{-1}\frac{\partial \eta(t)}{\partial a(0)}$. Similarly, $\frac{d}{dt}\frac{\partial a(t)}{\partial \eta(0)}=m^{-1}\frac{\partial \eta(t)}{\partial \eta(0)}$. Using these two facts, we can compute $\frac{dA}{dt}(t)$ by differentiating (1.11). Substituting the result in Eq. (1.8), we obtain Eq. (1.12).

We now turn to the proof of (1.5). There exists a constant R_1 (clearly independent of $\hbar$!) such that $|a(t)|<R_1/2$ whenever $|t|\leqq T$. Also, Eq. (1.11) shows that there exists R_2 such that $\|A(t)\|\leqq\hbar^{-p}R_2/2$ for $|t|\leqq T$ and $\hbar\leqq 1$, where $p=\mathrm{Max}\{0,2\alpha-1\}$.

Since $\lambda>0$, some arithmetic shows that α, p, and $\gamma=(\lambda+1)/3$ satisfy $\alpha>p$ and $\gamma\in(0,\alpha-p)$. So, by Lemma 2.3, there exist C and $\delta>0$ such that $\hbar<\delta$, $|a|<R_1$, $f\in L^\infty(\mathbb{R}^n)$, and $\|A\|\leqq R_2\hbar^{-p}$ imply

$$\|(e^{-isV/\hbar}-e^{-isW_a/\hbar})f\psi_\alpha(A,B,\hbar,a,\eta,\cdot)\|\leqq C\|f\|_\infty|s|\hbar^\lambda/3T, \tag{2.3}$$

where $W_a(x)=V(a)+\langle V^{(1)}(a),(x-a)\rangle+\frac{1}{2}\langle(x-a),V^{(2)}(a)(x-a)\rangle$.

For the Remainder of the Proof, we fix $\hbar<\delta$ and $t\in[-T,T]$.

By using the Trotter product formula and Eq. (2.3) in tandem, we will be led to the following discrete time analogs of the solution to Eqs. (1.6)–(1.10): For $1\leqq n\leqq N$, we define $a_N(0)=a(0)$, $\eta_N(0)=\eta(0)$, $A_N(0)=A(0)$, $B_N(0)=B(0)$, $S_N(0)=0$,

$$\eta_N(n)=\eta(0)-\sum_{j=1}^{n} V^{(1)}(a_N(j-1))\,t/N\,,$$

$$a_N(n)=a(0)+\sum_{j=1}^{n}\eta_N(j)\,t/Nm$$

$$A_N(n)=A(0)+\sum_{j=1}^{n} i\hbar^{1-2\alpha}B_N(j)\,t/2Nm$$

$$B_N(n)=B(0)+\sum_{j=1}^{n} 2i\hbar^{2\alpha-1}V^{(2)}(a_N(j-1))A_N(j-1)t/N\,,$$

and

$$S_N(n)=\sum_{j=1}^{n}[(\eta_N(j))^2/2m-V(a_N(j-1))]t/N\,.$$

Our conditions on V imply that by taking N very large we can make

$$|a(nt/N)-a_N(n)|+|\eta(nt/N)-\eta_N(n)|+\|A(nt/N)-A_N(n)\| + \|B(nt/N)-B_N(n)\|+|S(nt/N)-S_N(n)|$$

arbitrarily small for all $n=1,2,\ldots,N$ (see e.g., [2, Sect. VII.12]). So, by Lemma 2.1 and the dominated convergence theorem, there exists N_1 such that $N>N_1$ implies for $n\leqq N$, that $(A_N(n))^{-1}$ exists, $|a_N(n)|<R_1$, $\|A_N(n)\|<R_2\hbar^{-p}$, and

$$\|e^{iS_N(N)/\hbar}\varphi_\alpha(A_N(N),B_N(N),\hbar,a_N(N),\eta_N(N),\,\cdot\,) - e^{iS(t)/\hbar}\varphi_\alpha(A(t),B(t),\hbar,a(t),\eta(t),\,\cdot\,)\|<C\hbar^\lambda/3\,. \tag{2.4}$$

The Trotter product formula [11] shows the existence of N_2 such that $N>N_2$ implies

$$\|(e^{-itH(\hbar)/\hbar}-[e^{-itH_0(\hbar)/N\hbar}e^{-itV/N\hbar}]^N)\,\varphi_\alpha(A(0),B(0),\hbar,a(0),\eta(0),\,\cdot\,)\|<C\hbar^\lambda/3\,. \tag{2.5}$$

Now suppose $N>\mathrm{Max}\{N_1,N_2\}$. Since $\hbar<\delta$, $|a_N(0)|<R_1$, and $\|A_N(0)\|<R_2\hbar^{-p}$, inequality (2.3) shows

$$\|(e^{-itV/N\hbar}-e^{-itW_{a(0)}/N\hbar})\varphi_\alpha(A(0),B(0),\hbar,a(0),\eta(0),\,\cdot\,)\|<C\hbar^\lambda/3N\,.$$

Hence,

$$\|(e^{-itH_0(\hbar)/N\hbar}e^{-itV/N\hbar}-e^{-itH_0(\hbar)/N\hbar}e^{-itW_{a(0)}/N\hbar}),\ \varphi_\alpha(A(0),B(0),\hbar,a(0),\eta(0),\,\cdot\,)\|<C\hbar^\lambda/3N\,.$$

However, Lemma 2.2 shows

$$[e^{-itH_0(\hbar)/N\hbar}e^{-itW_{a(0)}/N\hbar}]\,\varphi_\alpha(A(0),B(0),\hbar,a(0),\eta(0),x) = e^{iS_N(1)/\hbar}\varphi_\alpha(A_N(1),B_N(1),\hbar,a_N(1),\eta_N(1),x)\,.$$

By our choice of N, we may iterate this procedure to obtain

$$\left\| \prod_{j=1}^{n} [e^{-itH_0(\hbar)/N\hbar} e^{-itV/N\hbar}] \psi_\alpha(A(0), B(0), h, a(0), \eta(0), \cdot) - e^{iS_N(n)/\hbar} \psi_\alpha(A_N(n), B_N(n), \hbar, a_N(n), \eta_N(n), \cdot) \right\| < nC\hbar^\lambda/3N \tag{2.6}$$

for $n=1,2,\ldots,N$. In particular, this holds for $n=N$.

The proof is now completed by combining inequalities (2.4), (2.5), and (2.6). □

3. Scattering Theory

The purpose of this section is to prove Theorem 1.2. Although the proof of this theorem is similar to that of Theorem 1.1, it requires two lemmas which are not in Sect. 2. Lemma 3.1 establishes properties of solutions of Eqs. (1.6)–(1.10) for infinite times. Lemma 3.2 is the infinite time analog of Lemma 2.3.

Lemma 3.1. *Suppose* $\hbar>0$ *and* $\alpha\in(0,1)$. *For some* $\nu>0$, *assume* $V\in C^3(\mathbb{R}^n)$ *satisfies*

$$\|V^{(j)}(x)\| \leqq c_j(1+|x|)^{-1-j-\nu} \quad \textit{for} \quad 0\leqq j\leqq 3.$$

Let $a_-\in\mathbb{R}^n$, $\eta_-\in\mathbb{R}^n$, *and let* A_- *and* B_- *be any two complex* $n\times n$ *matrices. If* $\eta_-\neq 0$, *then there exists a unique solution* $[A(t), B(t), a(t), \eta(t), S(t)]$ *to the system* (1.6)–(1.10) *such that* (1.13), (1.14), (1.17_-), (1.18_-), (1.19), (1.21), *and* (1.22) *hold. If* $(a_-,\eta_-)\notin\mathscr{E}$, *then there exist* $\eta_+\neq 0$ *and* a_+ *such that* (1.15), (1.16), (1.17_+), (1.18_+), (1.20), (1.23), *and* (1.24) *also hold. Furthermore, if* $(a_-,\eta_-)\notin\mathscr{E}$ *and* A_- *and* B_- *satisfy conditions* (1.1)–(1.4), *then the pair* $A(t)$, $B(t)$ *and the pair* A_+, B_+ *also satisfy conditions* (1.1)–(1.4).

Proof. Simon [14, Theorem 2] has shown that given a_- and $\eta_-\neq 0$, there exists a unique solution $[a(t),\eta(t)]$ to (1.6) and (1.7) which satisfies (1.13) and (1.14). Explicitly, this solution satisfies

$$a(t)=a_-+t\eta_-/m-m^{-1}\int_{-\infty}^{t} ds \int_{-\infty}^{s} V^{(1)}(a(r))dr \tag{3.1}$$

and

$$\eta(t)=\eta_- - \int_{-\infty}^{t} V^{(1)}(a(s))ds. \tag{3.2}$$

Using the idea of Theorem 3 of [14], our hypotheses on V and Theorem 9.4 of [9] show that $\frac{\partial a(t)}{\partial a_-}$, $\frac{\partial a(t)}{\partial \eta_-}$, $\frac{\partial \eta(t)}{\partial a_-}$, and $\frac{\partial \eta(t)}{\partial \eta_-}$ exist and satisfy

$$\frac{\partial a(t)}{\partial a_-}=I-m^{-1}\int_{-\infty}^{t} ds \int_{-\infty}^{s} V^{(2)}(a(r))\frac{\partial a(r)}{\partial a_-}dr, \tag{3.3}$$

$$\frac{\partial a(t)}{\partial \eta_-}=t/m-m^{-1}\int_{-\infty}^{t} ds \int_{-\infty}^{s} V^{(2)}(a(r))\frac{\partial a(r)}{\partial \eta_-}dr, \tag{3.4}$$

$$\frac{\partial \eta(t)}{\partial a_-}=-\int_{-\infty}^{t} V^{(2)}(a(s))\frac{\partial a(s)}{\partial a_-}ds, \tag{3.5}$$

and

$$\frac{\partial\eta(t)}{\partial\eta_-}=I-\int_{-\infty}^{t} V^{(2)}(a(s))\frac{\partial a(s)}{\partial\eta_-}ds. \tag{3.6}$$

If $(a_-,\eta_-)\notin\mathscr{E}$, then [8; 13; 14, Theorem 5] there exist a_+ and $\eta_+\neq 0$ such that (1.15) and (1.16) are satisfied. From Eq. (3.2) we see that

$$\eta_+=\eta_- -\int_{-\infty}^{\infty} V^{(1)}(a(s))ds. \tag{3.7}$$

Using this and Eq. (3.1), we have

$$\begin{aligned} a(t)&=a_-+t\eta_+/m+tm^{-1}\int_{-\infty}^{\infty} V^{(1)}(a(r))dr-m^{-1}\int_{-\infty}^{t} ds\int_{-\infty}^{s} V^{(1)}(a(r))dr\\ &=a_-+t\eta_+/m+m^{-1}\int_0^t ds\int_{-\infty}^{\infty} V^{(1)}(a(r))dr-m^{-1}\int_0^t ds\int_{-\infty}^{s} V^{(1)}(a(r))dr\\ &\quad -m^{-1}\int_{-\infty}^{0} ds\int_{-\infty}^{s} V^{(1)}(a(r))dr\\ &=a_- -m^{-1}\int_{-\infty}^{0} ds\int_{-\infty}^{s} V^{(1)}(a(r))dr+m^{-1}\int_0^t ds\int_s^{\infty} V^{(1)}(a(r))dr+t\eta_+/m. \end{aligned}$$

Letting t tend to infinity in this expression, we obtain a formula for a_+:

$$a_+=a_- -m^{-1}\int_{-\infty}^{0} ds\int_{-\infty}^{s} V^{(1)}(a(r))dr+m^{-1}\int_0^{\infty} ds\int_s^{\infty} V^{(1)}(a(r))dr. \tag{3.8}$$

Energy conservation requires $(\eta_-)^2/2m=(\eta(s))^2/2m+V(a(s))$ for all s.

Thus,

$$\begin{aligned} S(t)&=t(\eta_-)^2/2m-2\int_{-\infty}^{t} V(a(s))ds\\ &=t(\eta_-)^2/2m+\int_{-\infty}^{t} [(\eta(s))^2/2m-(\eta_-)^2/2m-V(a(s))]ds \end{aligned}$$

is well defined and satisfies (1.10) and (1.19). If $(a_-,\eta_-)\notin\mathscr{E}$, then (1.15) and the hypotheses on V show that (1.20) holds with

$$S_+=-2\int_{-\infty}^{\infty} V(a(s))ds.$$

By standard existence and uniqueness theorems [2], we need only show existence and uniqueness of $A(t)$ and $B(t)$ on $(-\infty,-T)$ for some T. Let $Z(t)$ be any continuous $n\times n$ matrix valued function satisfying $\|Z\|_\infty=\sup_{t\in\mathbb{R}}\|Z(t)\|\leqq 1$. Then Eq. (1.15) and the hypotheses on V show that the integral

$$[\mathscr{G}Z](t)=-m^{-1}\int_{-\infty}^{t} ds\int_{-\infty}^{s} V^{(2)}(a(r))[A_-+i\hbar^{1-2\alpha}rB_-/2m+Z(r)]dr$$

is bounded by a Z-independent multiple of $|t|^{-\nu}$ for $t<0$. So, by taking T very large, we see that $\mathscr{G}$ is a strict contraction on $\mathscr{A}=\left\{Z:\|Z\|_{(-T)}=\sup_{t<-T}\|Z(t)\|\leqq 1\right\}$.

Thus, there exists a unique solution $Z\in\mathscr{A}$ to $Z=\mathscr{G}Z$. This solution is clearly differentiable, and

$$[A(t)=A_-+i\hbar^{1-2\alpha}tB_-/2m+Z(t), B(t)=B_--2im\hbar^{2\alpha-1}Z'(t), a(t), \eta(t), S(t)]$$

is the unique solution to (1.6)–(1.10) which satisfies (1.13). (1.14), (1.17_-), (1.18_-), and (1.19).

If $(a_-,\eta_-)\notin\mathscr{E}$, then we can reverse time in the above argument and produce a mapping $\Lambda:(A_+,B_+)\to(A(\cdot),B(\cdot))$ which is linear and injective. Since the space of solutions of (1.8) and (1.9) has the same dimension as the space of asymptotes $\{(A_+,B_+)\}$, Λ is surjective, and hence, invertible. Therefore, our solution $[A(t), B(t)]$ satisfies (1.17_+) and (1.18_+) for some A_+ and B_+.

Next we turn to the proof of Eqs. (1.21) and (1.22). From (3.3) and (3.4) we see that $\dfrac{\partial a(t)}{\partial a_-}$ and $\dfrac{\partial a(t)}{\partial \eta_-}$ are two independent solutions to the linear equation $\dfrac{d^2f}{dt^2}(t)=-m^{-1}V^{(2)}(a(t))f(t)$. Equations (1.8) and (1.9) show that $A(t)$ also satisfies this equation. Consequently, (1.21) holds since the right hand and left hand sides have the same asymptotic behavior as $t\to-\infty$. Equation (1.22) now follows from (1.21) in the same way that (1.12) followed from (1.11) in the proof of Theorem 1.1.

To prove (1.23) and (1.24), we assume $(a_-,\eta_-)\notin\mathscr{E}$ and note that we have already shown that $A(t)$, $\dfrac{\partial a(t)}{\partial a_-}$, and $\dfrac{\partial a(t)}{\partial \eta_-}$ satisfy the same differential equation. Furthermore, in our proof of the existence of A_+ and B_+, we completely analyzed the asymptotic behavior of all solutions to that equation. Thus, $\left\|\dfrac{\partial a(t)}{\partial a_-}\right\|$ and $\left\|\dfrac{\partial a(t)}{\partial \eta_-}\right\|$ grow at most like constant multiples of t as $t\to\infty$. Using this, we can differentiate (3.7) and (3.8) to prove that $\dfrac{\partial a_+}{\partial a_-}$, $\dfrac{\partial a_+}{\partial \eta_-}$, $\dfrac{\partial \eta_+}{\partial a_-}$, and $\dfrac{\partial \eta_+}{\partial \eta_-}$ exist and satisfy

$$\frac{\partial\eta_+}{\partial a_-}=-\int_{-\infty}^{\infty}V^{(2)}(a(s))\frac{\partial a(s)}{\partial a_-}ds\,, \tag{3.9}$$

$$\frac{\partial\eta_+}{\partial \eta_-}=I-\int_{-\infty}^{\infty}V^{(2)}(a(s))\frac{\partial a(s)}{\partial \eta_-}ds\,, \tag{3.10}$$

$$\frac{\partial a_+}{\partial a_-}=I-m^{-1}\int_{-\infty}^{0}ds\int_{-\infty}^{s}V^{(2)}(a(r))\frac{\partial a(r)}{\partial a_-}dr+m^{-1}\int_{0}^{\infty}ds\int_{s}^{\infty}V^{(2)}(a(r))\frac{\partial a(r)}{\partial a_-}dr\,, \tag{3.11}$$

and

$$\frac{\partial a_+}{\partial \eta_-}=-m^{-1}\int_{-\infty}^{0}ds\int_{-\infty}^{s}V^{(2)}(a(r))\frac{\partial a(r)}{\partial \eta_-}dr+m^{-1}\int_{0}^{\infty}ds\int_{s}^{\infty}V^{(2)}(a(r))\frac{\partial a(r)}{\partial \eta_-}dr\,. \tag{3.12}$$

Substituting (3.3) and (3.4) into (1.21) and using (3.9)–(3.11), we see that $A(t)$ is asymptotic to

$$\frac{\partial a_+}{\partial a_-}A_-+\tfrac{1}{2}i\hbar^{1-2\alpha}\frac{\partial a_+}{\partial \eta_-}B_-+\frac{t}{m}\left(\frac{\partial\eta_+}{\partial a_-}A_-+\tfrac{1}{2}i\hbar^{1-2\alpha}\frac{\partial\eta_+}{\partial\eta_-}B_-\right).$$

Similarly, by combining (1.22), (3.5), (3.6), (3.9), and (3.10) we see that

$$\lim_{t\to\infty}B(t)=\frac{\partial\eta_+}{\partial\eta_-}B_--2i\hbar^{2\alpha-1}\frac{\partial\eta_+}{\partial a_-}A_-\,.$$

These results imply (1.23) and (1.24).

Finally, let $(a_-, \eta_-) \notin \mathscr{E}$, and suppose A_- and B_- satisfy conditions (1.1)–(1.4). The proof of Lemma 2.1 clearly shows that there exist constant matrices C_1 and C_2 such that $B(t)^* A(t) + A(t)^* B(t) = C_1$ and $B(t)^t A(t) - A(t)^t B(t) = C_2$. Thus,

$$B(t)^*[A(t) - i\hbar^{1-2\alpha} tB(t)/2m] + [A(t) - i\hbar^{1-2\alpha} tB(t)/2m]^* B(t) = C_1$$

and

$$B(t)^t\, [A(t) - i\hbar^{1-2\alpha} tB(t)/2m] - [A(t) - i\hbar^{1-2\alpha} tB(t)/2m]^t\, B(t) = C_2 .$$

However, by using $\|V^{(2)}(x)\| \leqq c_2(1+|x|)^{-3-\nu}$ and Eqs. (1.21), (1.22), and (3.3)–(3.6), we see that $\lim_{t\to-\infty} A(t) - i\hbar^{1-2\alpha} tB(t)/2m = A_-$. Thus, $C_1 = B_-^* A_- + A_-^* B_-$ and $C_2 = B_-^t A_- - A_-^t B_-$. Since A_- and B_- satisfy (1.1)–(1.4), the proof of Lemma 2.1 shows that $C_1 = 2I$ and $C_2 = 0$. The proof of Lemma 2.1 now shows that $A(t)$ and $B(t)$ satisfy conditions (1.1)–(1.4) for all t.

By using the hypothesis $\|V^{(2)}(x)\| \leqq c_2(1+|x|)^{-3-\nu}$, our growth estimates on $\left\|\frac{\partial a(t)}{\partial a_-}\right\|$ and $\left\|\frac{\partial a(t)}{\partial \eta_-}\right\|$, Eqs. (1.21)–(1.24), (3.3)–(3.6), and (3.9)–(3.12), we can show that $\lim_{t\to+\infty} A(t) - i\hbar^{1-2\alpha} tB(t)/2m = A_+$. It follows that $B_+^* A_+ + A_+^* B_+ = C_1 = 2I$ and $B_+^t A_+ - A_+^t B_+ = C_2 = 0$. The proof of Lemma 2.1 now shows that A_+ and B_+ satisfy (1.1)–(1.4). □

Remark. Toward the end of the above proof, we noted that Eqs. (1.21)–(1.24), (3.3)–(3.6), and (3.9)–(3.12) show that

$$\lim_{t\to\pm\infty} A(t) - i\hbar^{1-2\alpha} tB(t)/2m = A_\pm . \tag{3.13}$$

Similarly, Eqs. (3.1), (3.2), (3.7), and (3.8) can be used to show that

$$\lim_{t\to\pm\infty} a(t) - t\eta(t)/m = a_\pm . \tag{3.14}$$

This statement is already implicitly contained in [14].

Also, Eqs. (3.2) and (3.7) and the formulas for $S(t)$ and S_+ show that

$$\lim_{t\to+\infty} S(t) - t|\eta(t)|^2/2m = S_+ . \tag{3.15}$$

Lemma 3.2. *Let the dimension of space be* $n \geqq 3$. *Let* $\alpha \in (1/3, 2/3)$ *and* $f \in L^\infty(\mathbb{R}^n)$. *For some* $\nu > 0$ *assume* $V \in C^3(\mathbb{R}^n)$ *satisfies*

$$\|V^{(j)}(x)\| \leqq c_j(1+|x|)^{-1-j-\nu} \quad \textit{for} \quad 0 \leqq j \leqq 3 .$$

Given $(a_-, \eta_-) \notin \mathscr{E}$, *and* A_- *and* B_- *satisfying conditions* (1.1)–(1.4), *let* $[A(t), B(t), a(t), \eta(t), S(t)]$ *be the solution to Eqs.* (1.6)–(1.10) *constructed in Lemma 3.1. If we define* $W_y(x)$ *by*

$$W_y(x) = V(y) + \langle V^{(1)}(y), (x-y)\rangle + \tfrac{1}{2}\langle (x-y), V^{(2)}(y)\,(x-y)\rangle ,$$

then for each positive $\lambda<\mathrm{Min}\{3\alpha-1,\ 2-3\alpha\}$, *there exists a positive continuous function* $F(t)\leqq C(1+|t|)^{-1-\nu/2}$, *such that* $\hbar\leqq 1$ *implies*

$$\|(e^{-isV/\hbar}-e^{-isW_{a(t)}/\hbar})f\psi_\alpha(A(t),B(t),\hbar,a(t),\eta(t),\ \cdot)\|\leqq F(t)\,\|f\|_\infty|s|\hbar^\lambda.$$

Proof. Suppose $\mu<1$ and $|x-y|\leqq\mu(1+|y|)$. Let z be the element of $\{z=rx+(1-r)y:0\leqq r\leqq 1\}$ which minimizes $|z|$. Then by the triangle inequality,

$$\begin{aligned}\|V^{(2)}(x)-V^{(2)}(y)\|&\leqq c_3(1+|z|)^{-4-\nu}|x-y|\\&\leqq c_3(1+|y|-|y-z|)^{-4-\nu}|x-y|\\&\leqq c_3(1+|y|-\mu(1+|y|))^{-4-\nu}|x-y|.\end{aligned}$$

So, if we set $\beta(y)=c_3(1-\mu)^{-4-\nu}(1+|y|)^{-4-\nu}$, then $|x-y|\leqq\mu(1+|y|)$ implies $\|V^{(2)}(x)-V^{(2)}(y)\|\leqq\beta(y)|x-y)$. From this, it follows that $|x-y|\leqq\mu(1+|y|)$ implies $|V(x)-W_y(x)|\leqq\beta(y)|x-y|^3/6$.

Let $X_1(\hbar,y,\cdot)$ and $X_2(\hbar,y,\cdot)$ denote the characteristic functions of $\{x:|x-y|\leqq\hbar^{(\lambda+1)/3}\mu(1+|y|)\}$ and $\{x:|x-y|>\hbar^{(\lambda+1)/3}\mu(1+|y|)\}$, respectively. Then, for $\hbar\leqq 1$,

$$\begin{aligned}&\|(e^{-isV/\hbar}-e^{-isW_{a(t)}/\hbar})f\psi_\alpha(A(t),B(t),\hbar,a(t),\eta(t),\ \cdot)\|\\&\leqq\|f\|_\infty\hbar^{-1}|s|\,\||V-W_{a(t)}|\psi_\alpha(A(t),B(t),\hbar,a(t),\eta(t),\ \cdot)\|\\&\leqq\|f\|_\infty\hbar^{-1}|s|\{\|X_1(\hbar,a(t),\ \cdot)|V-W_{a(t)}|\psi_\alpha(A(t),B(t),\hbar,a(t),\eta(t),\ \cdot)\|\\&\quad+\|X_2(\hbar,a(t),\ \cdot)|V-W_{a(t)}|\psi_\alpha(A(t),B(t),\hbar,a(t),\eta(t),\ \cdot)\|\}\\&\leqq\|f\|_\infty\hbar^{-1}|s|\{\beta(a(t))\mu^3\hbar^{\lambda+1}(1+|a(t)|)^3\\&\quad+\|X_2(\hbar,a(t),\ \cdot)V\psi_\alpha(A(t),B(t),\hbar,a(t),\eta(t),\ \cdot)\|\\&\quad+\|X_2(\hbar,a(t),\ \cdot)W_{a(t)}\psi_\alpha(A(t),B(t),\hbar,a(t),\eta(t),\ \cdot)\|\}\\&=\|f\|_\infty\hbar^{-1}|s|\{I(t)+II(t)+III(t)\}.\end{aligned}$$

The asymptotics of $a(t)$ guarantee the existence of a positive continuous function $F_1(t)\leqq C_1(1+|t|)^{-1-\nu}$, such that $|I(t)|\leqq F_1(t)\hbar^{(\lambda+1)}$.

By Hölder's inequality, $II(t)$ is bounded by

$$\begin{aligned}&\|X_2(\hbar,a(t),x)\exp\{-(8\hbar^{2\alpha})^{-1}\langle(x-a(t)),\mathrm{Re}\,B(t)A(t)^{-1}(x-a(t))\rangle\}\|_\infty\\&\quad\cdot\|V\|_p\,\|(2\pi)^{-n/4}\hbar^{-n\alpha/2}(\det A(t))^{-1/2}\exp\{-(8\hbar^{2\alpha})^{-1}\\&\cdot\langle(x-a(t)),\mathrm{Re}\,B(t)A(t)^{-1}(x-a(t))\rangle\}\|_q,\end{aligned}\tag{3.16}$$

where $p^{-1}+q^{-1}=1/2$.

Since $A(t)$ and $B(t)$ satisfy conditions (1.1)–(1.4), the first factor of (3.16) is bounded by $\exp\{-(8\hbar^{2\alpha})^{-1}\|A(t)\|^{-2}[\hbar^{(\lambda+1)/3}\mu(1+|a(t)|)]^2\}$. The continuity and asymptotics of $a(t)$ and $A(t)$ show that this is bounded by $\exp\{-C'\hbar^{-\varepsilon}\}$, where C' is some constant independent of $\hbar$ and t, and $\varepsilon=2(\alpha-(\lambda+1)/3)$. Our hypotheses on α and λ guarantee $\varepsilon>0$. By interpolation between $q=2$ and $q=\infty$, the third factor of (3.16) is bounded by some $\hbar$-independent multiple of $(\hbar^{n\alpha}|\det A(t)|)^{1/q-1/2}$ for $2\leqq q\leqq\infty$. Since $n\geqq 3$, our hypotheses on V guarantee the existence of some $p<n(1+\nu/2)^{-1}$ such that $\|V\|_p<\infty$. Making such a choice for p, we see that $II(t)$ is bounded by a multiple of $(\hbar^{n\alpha}|\det A(t)|)^{-1/p}\exp\{-C'\hbar^{-\varepsilon}\}$. So, the continuity and asymptotics of $A(t)$ show the existence of a positive continuous function $F_2(t) \leqq C_2(1+|t|)^{-1-\nu/2}$ such that $|II(t)| \leqq F_2(t)\hbar^{\lambda+1}$.

$III(t)$ is bounded by a sum of three terms:

$$\begin{aligned} III(t) \leqq & |V(a(t))| \, \|X_2(\hbar, a(t), \cdot)\psi_\alpha(A(t), B(t), \hbar, a(t), \eta(t), \cdot)\| \\ & + |V^{(1)}(a(t))| \, \|X_2(\hbar, a(t), x)|x-a(t)|\psi_\alpha(A(t), B(t), \hbar, a(t), \eta(t), x)\| \\ & + \tfrac{1}{2}\|V^{(2)}(a(t))\| \, \|X_2(\hbar, a(t), x)|x-a(t)|^2\psi_\alpha(A(t), B(t), \hbar, a(t), \eta(t), x)\| . \end{aligned}$$

By the analysis used to control $II(t)$, this sum is bounded by

$$\begin{aligned} & [|V(a(t))| \, \|\phi_\alpha(t, \hbar, x)\| + |V^{(1)}(a(t))| \| \, |x-a(t)| \, \phi_\alpha(t, \hbar, x)\| \\ & \qquad + \tfrac{1}{2}\|V^{(2)}(a(t))\| \, \| |x-a(t)|^2 \phi_\alpha(t, \hbar, x)\|] \exp\{-C\hbar^{-\varepsilon}\}, \end{aligned}$$

where

$$\begin{aligned} \phi_\alpha(t, \hbar, x) = & (2\pi)^{-n/4}\hbar^{-n\alpha/2}(\det A(t))^{-1/2} \\ & \cdot \exp\{-(8\hbar^{2\alpha})^{-1}\langle(x-a(t)), [A(t)A(t)^*]^{-1}(x-a(t))\rangle\} . \end{aligned}$$

We write the above L^2-norms as square roots of integrals, and then change the variable of integration to $z = A(t)^{-1}(x-a(t))$. This leads to the bound

$$\begin{aligned} III(t) \leqq & [|V(a(t))| D_1 + |V^{(1)}(a(t))| D_2 \|A(t)\| + \|V^{(2)}(a(t))\| \\ & \cdot D_3\|A(t)\|^2] \exp\{-C\hbar^{-\varepsilon}\}, \end{aligned}$$

where D_1, D_2, and D_3 are constants. The hypotheses on V and the asymptotics of $a(t)$ and $A(t)$ now show that $III(t)$ is bounded by $\hbar^{\lambda+1}F_3(t)$ for some positive continuous function $F_3(t) \leqq C_3(1+|t|)^{-1-\nu}$.

Setting $F = F_1 + F_2 + F_3$, the proof is complete. □

Proof of Theorem 1.2. Lemma 3.1 establishes everything we need except for Eqs. (1.25) and (1.26). Furthermore, by Lemma 2.2 and Eqs. (3.13)–(3.15),

$$\begin{aligned} & \lim_{t \to \infty} e^{-itH_0(\hbar)/\hbar} e^{iS(t)/\hbar} \psi_\alpha(A(t), B(t), \hbar, a(t), \eta(t), x) \\ & \quad = e^{iS_+/\hbar}\psi_\alpha(A_+, B_+, \hbar, a_+, \eta_+, x) . \end{aligned}$$

Thus, (1.25) implies (1.26).

To prove (1.25) we need only prove that given $\varepsilon > 0$, there exists T such that $s < -T$ implies that

$$\begin{aligned} & \|e^{-isH_0(\hbar)/\hbar}\psi_\alpha(A_-, B_-, \hbar, a_-, \eta_-, \cdot) \\ & \quad - e^{i(t-s)H(\hbar)/\hbar} e^{iS(t)/\hbar}\psi_\alpha(A(t), B(t), \hbar, a(t), \eta(t), \cdot)\| < C\hbar^\lambda + \varepsilon \end{aligned}$$

for all $t \in \mathbb{R}$.

By Lemmas 2.2 and 3.1, and the dominated convergence theorem, there exists T such that $s < -T$ implies

$$\begin{aligned} & \|e^{-isH_0(\hbar)/\hbar}\psi_\alpha(A_-, B_-, \hbar, a_-, \eta_-, \cdot) \\ & \quad - e^{iS(s)/\hbar}\psi_\alpha(A(s), B(s), \hbar, a(s), \eta(s), \cdot)\| < \varepsilon . \end{aligned}$$

Thus, it is sufficient to prove that for any t and s, there exists a C such that

$$\|e^{iS(s)/\hbar}\psi_\alpha(A(s),B(s),\hbar,a(s),\eta(s),\cdot) - e^{i(t-s)H(\hbar)/\hbar}e^{iS(t)/\hbar}\psi_\alpha(A(t),B(t),\hbar,a(t),\eta(t),\cdot)\| < C\hbar^\lambda.$$

To prove this, we simply repeat the Trotter product formula argument at the end of the proof of Theorem 1.1, with Lemma 2.3 replaced by Lemma 3.2. The value of C which we obtain is $\int_{-\infty}^{\infty} F(t)dt$, where $F\in L^1(\mathbb{R})$ is the function in the conclusion of Lemma 3.2. □

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Note added in proof. Ideas closely related to ours may be found in Heller, E.J.: Classical S-matrix limit of wave packet dynamics. J. Chem. Phys. **65**, 4979–4989 (1976).