Raising and Lowering Operators for Semiclassical Wave Packets

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Abstract

We construct raising and lowering operators for certain orthonormal bases of $L^2(\mathbb{R}^n)$. These bases consist of quantum mechanical wave packets that can be used to develop asymptotic expansions for solutions to the time–dependent Schrödinger equation in the semiclassical limit. With the knowledge of the raising and lowering operators, we simplify the construction of these bases and the proofs of their crucial properties. We also present simplified proofs of several results in semiclassical quantum mechanics.

* Supported in part by the National Science Foundation under grant number DMS–9703751.

1. Introduction

To study the semiclassical limit of quantum mechanics, the author constructed [13, 15] special orthonormal bases of $L^2(\mathbb{R}^n)$. Once these bases were constructed and their crucial properties established, it was easy [13, 15] to develop asymptotic expansions in powers of $\hbar^{1/2}$ for certain solutions to the time–dependent Schrödinger equation $i\,\hbar\,\frac{\partial\psi}{\partial t} \;=\; -\frac{\hbar^2}{2}\,\Delta\,\psi\,+\,V(x)\,\psi$. Other authors have subsequently used these wave packets for a variety of purposes [1–12, 14, 16–25, 27–32]. Furthermore, Combescure [7] has proved that these wave packets coincide with "generalized squeezed states" that have found widespread use in physics.

The constructions of the bases in [13, 15] are complicated, and some of their properties are proved by unituitive, brute–force techniques. Our present goal is to provide new constructions that are simpler and analogous to those for the eigenfunctions of the harmonic oscillator. This is accomplished by presenting operators for the semiclassical wave packets that are direct analogs of the standard raising and lowering operators for the familiar harmonic oscillator.

The paper is organized as follows: In Section 2 we present our results for the case of one space dimension. In Section 3 we present the general n–dimensional case. In Section 4 we give explicit formulas for all matrix elements of x^n in the bases constructed in Section 2.

2. The One–Dimensional Case

The one–dimensional case is simple and instructive, so we present it separately.

Throughout this section we assume $a\in\mathbb{R}$, $\eta\in\mathbb{R}$, $\hbar>0$, $A\in\mathbb{C}$, $B\in\mathbb{C}$, and the normalization condition

$$\overline{A}\,B\,+\,\overline{B}\,A\;=\;2. \tag{2.1}$$

Definition Let $p\;=\;-\,i\,\hbar\,\frac{\partial}{\partial x}$ be the momentum operator. We define raising and lowering operators from the Schwartz space $\mathcal{S}$ to itself by the formulas

$$\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)^*\;=\;\frac{1}{\sqrt{2\hbar}}\;\left[\;\overline{B}\;(\,x\;-\;a\,)\;-\;i\,\overline{A}\;\;(\,p\;-\;\eta\,)\;\right], \tag{2.2}$$

and

$$\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)\;\;=\;\frac{1}{\sqrt{2\hbar}}\;\left[\;B\;(\,x\;-\;a\,)\;+\;i\,A\;\;(\,p\;-\;\eta\,)\;\right]. \tag{2.3}$$

By a simple calculation, condition (2.1) implies

$$\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)\,\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)^*\;-\;\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)^*\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)\;=\;I. \tag{2.4}$$

Definition By solving the trivial first order linear ordinary differential equation,

$$\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)\,\varphi_0(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\;=\;0, \tag{2.5}$$

we see that 0 is a non–degenerate eigenvalue of $\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)$. Modulo a plus or minus sign, we fix the phase and normalization of the eigenvector $\varphi_0(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)$ by the formula

$$\varphi_0(A,\,B,\,\hbar,\,a,\,\eta,\,x)\;=\;\pi^{-1/4}\,\hbar^{-1/4}\,A^{-1/2}\,\exp\Big\{-BA^{-1}\,(x-a)^2/(2\hbar)\;+\;i\,\eta\,(x-a)/\hbar\Big\}. \tag{2.6}$$

We then define $\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)$ recursively by

$$\varphi_{k+1}(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\;=\;\frac{1}{\sqrt{k+1}}\,\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)^*\;\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot). \tag{2.7}$$

Remark 2.1 Formulas (2.5) and (2.7) define all the functions $\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)$, $k=0,\,1,\,2,\,\ldots$, modulo a single numerical phase. Our explicit formula (2.6) reduces the ambiguity to the choice of the sign of $A^{-1/2}$. The particular choice of that sign depends on the context.

Remark 2.2 From the form of $\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)^*$ and the explicit formula (2.6), we see that $\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,x)$ is a k^{th} degree polynomial in $\frac{x-a}{\sqrt{\hbar}}$ times $\varphi_0(A,\,B,\,\hbar,\,a,\,\eta,\,x)$.

Theorem 2.3 The functions $\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)$, $k=0,\,1,\,2,\,\ldots$, form an orthonormal basis of $L^2(\mathbb{R})$. They satisfy

$$\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)\;\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\;=\;\sqrt{k}\;\varphi_{k-1}(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot), \tag{2.8}$$

$$\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)^*\;\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\;=\;\sqrt{k+1}\;\varphi_{k+1}(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot), \tag{2.9}$$

$$\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)^*\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)\;\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\;=\;k\;\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot), \tag{2.10}$$

$$\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)^*\;\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\;=\;(k+1)\;\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot). \tag{2.11}$$

Proof: We first prove (2.8) by induction. For $k=0$, we have (2.5). For $k=1$, by (2.7), (2.4), and (2.5), we have

$$\begin{aligned}
\mathcal{A}\,\varphi_1 &= \mathcal{A}\,\mathcal{A}^*\,\varphi_0 \\
&= (\,\mathcal{A}\mathcal{A}^* - \mathcal{A}^*\mathcal{A}\,)\,\varphi_0 \\
&= \sqrt{1}\,\varphi_0.
\end{aligned}$$

For the induction step, we assume $k \geq 2$ and $\mathcal{A}\,\varphi_{k-1} = \sqrt{k-1}\,\varphi_{k-2}$. This, (2.7), and (2.4) imply

$$\begin{aligned}
\mathcal{A}\,\varphi_k &= \frac{1}{\sqrt{k}}\,\mathcal{A}\,\mathcal{A}^*\,\varphi_{k-1} \\
&= \frac{1}{\sqrt{k}}\,(\,\mathcal{A}\mathcal{A}^* - \mathcal{A}^*\mathcal{A}\,)\,\varphi_{k-1} + \frac{1}{\sqrt{k}}\,\mathcal{A}^*\mathcal{A}\varphi_{k-1} \\
&= \frac{1}{\sqrt{k}}\,\varphi_{k-1} + \frac{1}{\sqrt{k}}\,\mathcal{A}^*\sqrt{k-1}\,\varphi_{k-2} \\
&= \sqrt{k}\,\varphi_{k-1}.
\end{aligned}$$

This proves (2.8).

Formula (2.9) is just a restatement of (2.7). Formulas (2.10) and (2.11) follow immediately from (2.8) and (2.9).

Next, we prove inductively that $\|\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\,\| = 1$. For $k=0$ we do this directly from (2.6) using the relation $\mathrm{Re}\,BA^{-1} = |A|^{-2}$, which is equivalent to (2.1). Next, integrating by parts and using (2.5), we have

$$\begin{aligned}
\|\,\varphi_1\,\|^2 &= \langle\,\mathcal{A}^*\varphi_0,\,\mathcal{A}^*\varphi_0\,\rangle \\
&= \langle\,\varphi_0,\,\mathcal{A}\mathcal{A}^*\varphi_0\,\rangle \\
&= \langle\,\varphi_0,\,(\,\mathcal{A}\mathcal{A}^* - \mathcal{A}^*\mathcal{A}\,)\,\varphi_0\,\rangle \\
&= \langle\,\varphi_0,\,\varphi_0\,\rangle \\
&= 1.
\end{aligned}$$

For the induction step, assume $k \geq 2$ and $\|\,\varphi_{k-1}\,\| = \|\,\varphi_{k-2}\,\| = 1$. This, (2.7), (2.4), (2.8), and two integrations by parts yield

$$\begin{aligned}
\|\,\varphi_k\,\|^2 &= \frac{1}{k}\,\langle\,\mathcal{A}^*\,\varphi_{k-1},\,\mathcal{A}^*\,\varphi_{k-1}\,\rangle \\
&= \frac{1}{k}\,\langle\,\varphi_{k-1},\,\mathcal{A}\,\mathcal{A}^*\,\varphi_{k-1}\,\rangle \\
&= \frac{1}{k}\,\langle\,\varphi_{k-1},\,(\,\mathcal{A}\,\mathcal{A}^*\,-\,\mathcal{A}^*\,\mathcal{A}\,)\,\varphi_{k-1}\,\rangle\;+\;\frac{1}{k}\,\langle\,\varphi_{k-1},\,\mathcal{A}^*\,\mathcal{A}\,\varphi_{k-1}\,\rangle \\
&= \frac{1}{k}\,\langle\,\varphi_{k-1},\,\varphi_{k-1}\,\rangle\;+\;\frac{1}{k}\,\langle\,\mathcal{A}\,\varphi_{k-1},\,\mathcal{A}\,\varphi_{k-1}\,\rangle \\
&= \frac{1}{k}\;[\,1\,+\,(k-1)\,\langle\,\varphi_{k-2},\,\varphi_{k-2}\,\rangle\,] \\
&= 1.
\end{aligned}$$

Orthonormality of the φ_k now follows from (2.10) or (2.11) and the essential self–adjointness of $\mathcal{A}^*\,\mathcal{A}$ or $\mathcal{A}\,\mathcal{A}^*$. Completeness of the φ_k can be proved by mimicking standard proofs for the harmonic oscillator, where $A = B = 1$ and $a = \eta = 0$. ■

Remark 2.4 Theorem 2.3 allows us to explicitly diagonalize any quantum Hamiltonian of the form

$$H \;=\; \frac{1}{2}\,\left(\,\alpha\,p^2\,+\,\beta\,(x\,p\,+\,p\,x)\,+\gamma\,x^2\,\right),$$

that satisfies $\omega^2 \;=\; (\alpha\gamma - \beta^2) \;>\; 0$. This follows from writing

$$H \;=\; \frac{\hbar\,\omega}{2}\;(\,\mathcal{A}^*\,\mathcal{A}\,+\,\mathcal{A}\,\mathcal{A}^*\,),$$

where we have chosen $a = \eta = 0$, $A = \sqrt{\dfrac{\alpha}{\omega}}e^{i\theta}$, and $B = \sqrt{\dfrac{\gamma}{\omega}}e^{-i\theta}$, with $\theta \;=\; \dfrac{1}{2}\,\sin^{-1}\,\left(\dfrac{\beta}{\sqrt{\alpha\gamma}}\right)$. The eigenvalues and corresponding eigenvectors of H are $(k+\frac{1}{2})\hbar\omega$ and $\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)$ for $k = 0,\,1,\,2,\,\ldots.$

To transform wave functions from position space to momentum space, we use the scaled Fourier Transform

$$(\mathcal{F}_\hbar\psi)(\xi) \;=\; (2\pi\hbar)^{-1/2}\int_{\mathrm{I\!R}}\;\psi(x)\,e^{-i\xi x/\hbar}\,dx.$$

We have

$$\mathcal{F}_\hbar\;\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)\;{\mathcal{F}_\hbar}^{-1} \;=\; i\;\;\mathcal{A}(B,\,A,\,\hbar,\eta,-a) \tag{2.12}$$

and

$$\mathcal{F}_\hbar\;\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)^*\;{\mathcal{F}_\hbar}^{-1} \;=\; -\,i\;\;\mathcal{A}(B,\,A,\,\hbar,\eta,-a)^*. \tag{2.13}$$

From equations (2.5) and (2.12), it is clear that $(\mathcal{F}_\hbar\,\varphi_0(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot))(\xi)$ must be a ξ–independent phase times $\varphi_0(B,\,A,\,\hbar,\,\eta,\,-a,\,\xi)$. Explicit calculation of the phase shows

$$(\mathcal{F}_\hbar\,\varphi_0(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot))(\xi) \;=\; e^{-ia\eta/\hbar}\,\varphi_0(B,\,A,\,\hbar,\,\eta,\,-a,\,\xi). \tag{2.14}$$

From this and equations (2.7) and (2.13), we immediately have

$$(\mathcal{F}_\hbar\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot))(\xi) \;=\; (-i)^k\;e^{-ia\eta/\hbar}\;\varphi_k(B,\,A,\,\hbar,\,\eta,\,-a,\,\xi). \tag{2.15}$$

This result is Lemma 2.1 of [13]. The proof presented in [13] is a long, unituitive induction in k, based on two recursion formulas for Hermite polynomials.

The wave packets $\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)$ are particularly suited to the study of propagation generated by time–dependent Hamiltonians that are quadratic in position and momentum. For such systems, there is a close connection between classical and quantum mechanics. See, *e.g.*, [22]. Suppose $\alpha(\cdot)$, $\beta(\cdot)$, $\gamma(\cdot)$, $\delta(\cdot)$, $\epsilon(\cdot)$, and $\zeta(\cdot)$ are continuous, real-valued functions, and consider the classical Hamiltonian

$$H(x,p,t) \;=\; \frac{1}{2}\alpha(t)p^2\,+\,\beta(t)xp\,+\,\frac{1}{2}\gamma(t)x^2\,+\,\delta(t)p\,+\,\epsilon(t)x\,+\,\zeta(t).$$

Given any initial conditions $(A(0),\,B(0),\,a(0),\,\eta(0),\,S(0))$, there exists a unique solution $(A(t),\,B(t),\,a(t),\,\eta(t),\,S(t))$ to the system

$$\begin{aligned}
\dot{a}(t) &= \beta(t)\,a(t)\,+\,\alpha(t)\,\eta(t)\,+\,\delta(t)\\
\dot{\eta}(t) &= -\,\gamma(t)\,a(t)\,-\,\beta(t)\eta(t)\,-\,\epsilon(t)\\
\dot{A}(t) &= \beta(t)\,A(t)\,+\,i\,\alpha(t)\,B(t)\\
\dot{B}(t) &= i\,\gamma(t)\,A(t)\,-\,\beta(t)\,B(t)\\
\dot{S}(t) &= \alpha(t)\,\frac{\eta(t)^2}{2}\,-\,\gamma(t)\,\frac{a(t)^2}{2}\,-\,\epsilon(t)\,a(t)\,-\,\zeta(t).
\end{aligned} \tag{2.16}$$

The solutions to the equations for A and B can be written in terms of the derivative of the phase space flow associated with a and η. Explicitly, we have

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

One proves these formulas by observing that the left and right hand sides of the equations satisfy the same differential equations and same initial conditions.

For the corresponding quantum mechanical system, we have the following :

Theorem 2.5 Suppose $\alpha(\cdot)$, $\beta(\cdot)$, $\gamma(\cdot)$, $\delta(\cdot)$, $\epsilon(\cdot)$, and $\zeta(\cdot)$ are continuous, real-valued functions on $\mathbb{R}$. Let $(A(\cdot),\, B(\cdot),\, a(\cdot),\, \eta(\cdot),\, S(\cdot))$ be any solution to the system (2.16). Then, for every k,

$$\psi(\hbar,\, t) \;=\; e^{iS(t)/\hbar}\, \varphi_k(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, \cdot) \tag{2.17}$$

satisfies the Schrödinger equation

$$i\,\hbar\,\frac{\partial \psi}{\partial t} \;=\; H(t)\,\psi, \tag{2.18}$$

for the time–dependent quantum Hamiltonian

$$H(t) \;=\; -\,\frac{\alpha(t)\hbar^2}{2}\,\frac{\partial^2}{\partial x^2} \,-\, i\,\frac{\beta(t)\hbar}{2}\,\left\{x\,\frac{\partial}{\partial x} \,+\, \frac{\partial}{\partial x}\,x\right\} \,+\, \frac{\gamma(t)}{2}\,x^2 \,-\, i\hbar\,\delta(t)\,\frac{\partial}{\partial x} \,+\, \epsilon(t)\,x \,+\, \zeta(t). \tag{2.19}$$

Proof: We prove this by a simple induction on k.

Fix $(A(0),\, B(0),\, a(0),\, \eta(0),\, S(0))$ and let $(A(t),\, B(t),\, a(t),\, \eta(t),\, S(t))$ be the corresponding solution to equation (2.16).

To initiate the induction, we verify by explicit calculation that
$\psi(\hbar,\, t) \;=\; e^{iS(t)/\hbar}\, \varphi_0(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, \cdot)$ satisfies the Schrödinger equation (2.18).

To do the induction step, we begin with another explicit calculation, to verify that as operators from $\mathcal{S}$ to $\mathcal{S}$, $\mathcal{A}^*(t) \;=\; \mathcal{A}(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t))^*$ satisfies

$$i\,\hbar\,\frac{\partial \mathcal{A}^*}{\partial t} \;=\; [\,\mathcal{A}^*(t),\, H(t)\,]\,. \tag{2.20}$$

We use equation (2.7) to write

$$\begin{aligned} &e^{iS(t)/\hbar}\, \varphi_{k+1}(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, \cdot) \\ &\qquad = \;\frac{1}{\sqrt{k+1}}\; \mathcal{A}(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t))^*\; e^{iS(t)/\hbar}\, \varphi_k(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, \cdot). \end{aligned}$$

By equation (2.20) and the product rule for differentiation, it follows that if
$e^{iS(t)/\hbar}\, \varphi_k(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, \cdot)$ satisfies equation (2.18), then
$e^{iS(t)/\hbar}\, \varphi_{k+1}(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, \cdot)$ does also. ■

Corollary 2.6 There exists a unique unitary propagator $U_\hbar(t,\, s)$ for the time–dependent quantum Hamiltonian (2.19) that satisfies

$$U(t,\, s)\, :\, \mathcal{S}\, \to\, \mathcal{S}$$

and

$$U_\hbar(t,\, s)\, e^{iS(s)/\hbar}\, \varphi_k(A(s),\, B(s),\, \hbar,\, a(s),\, \eta(s),\, \cdot)\; =\; e^{iS(t)/\hbar}\, \varphi_k(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, \cdot), \tag{2.21}$$

for all k and all solutions $(A(t),\, B(t),\, a(t),\, \eta(t),\, S(t))$ to the system (2.16).

Proof: To prove existence, we fix a particular solution $(A(t),\, B(t),\, a(t),\, \eta(t),\, S(t))$ to the system (2.16). We then use (2.21) and linearity to define $U_\hbar(t,\, s)$. Unitarity of $U_\hbar(t,\, s)$ follows from the orthogonality of the $\varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot)$.

As is the case for the standard Harmonic oscillator eigenstates [26], a function $\psi(x)$ belongs to $\mathcal{S}$ if and only if it has an expansion of the form

$$\psi(x)\; =\; \sum_{k=0}^{\infty}\, b_k\, \varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, x),$$

where the coefficients b_k decay faster than k^{-N} for all N. From this and (2.21), it follows that $U_\hbar(t,\, s)$ maps $\mathcal{S}$ to itself.

Since the functions of the form (2.17) satisfy (2.18), we also see that, as maps from $\mathcal{S}$ to itself, we have

$$i\,\hbar\, \frac{\partial}{\partial t}\, U_\hbar(t,\, s)\; =\; H(t)\, U_\hbar(t,\, s).$$

Uniqueness of $U_\hbar(t,\, s)$ follows from this equation and unitarity since if there were two such propagators, $U_{1,\hbar}(t,\, s)$ and $U_{2,\hbar}(t,\, s)$, then the t–derivative of

$$\langle\, U_{1,\hbar}(t,\, s)\, \psi_1,\; U_{2,\hbar}(t,\, s)\psi_2\, \rangle$$

would have to be zero for all $\psi_j\, \in\, \mathcal{S}$, and $U_{1,\hbar}(t,\, s)^*$ would have to be the inverse of $U_{2,\hbar}(t,\, s)$. Because of this uniqueness, we obtain the same propagator, regardless of which particular solution of the system (2.16) we use to define $U_\hbar(t,\, s)$. Thus, equation (2.21) holds for all solutions $(A(t),\, B(t),\, a(t),\, \eta(t),\, S(t))$ to the system (2.16). ■

We next note that on $\mathcal{S}$,

$$x\, -\, a\; =\; \sqrt{\frac{\hbar}{2}}\; \left(A\, \mathcal{A}(A,\, B,\, \hbar,\, a, \eta)^*\, +\, \overline{A}\, \mathcal{A}(A,\, B,\, \hbar,\, a, \eta)\right), \tag{2.22}$$

and

$$p - \eta \;=\; i\sqrt{\frac{\hbar}{2}}\;\left(B\,\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)^* \;-\; \overline{B}\,\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)\right). \tag{2.23}$$

From these relations, (2.8), (2.9), and the orthonormality of the φ_k, we see that

$$\|\,(x-a)\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\,\| \;=\; \left(\frac{\hbar}{2}\right)^{1/2}\,|A|\,\sqrt{2k+1}, \tag{2.24}$$

$$\|\,(x-a)^2\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\,\| \;=\; \left(\frac{\hbar}{2}\right)\,|A|^2\,\sqrt{6k^2+6k+3}, \tag{2.25}$$

$$\|\,(x-a)^3\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\,\| \;=\; \left(\frac{\hbar}{2}\right)^{3/2}\,|A|^3\,\sqrt{20k^3+30k^2+40k+15}, \tag{2.26}$$

and in general,

$$\|\,(x-a)^m\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\,\| \;=\; \left(\frac{\hbar}{2}\right)^{m/2}\,|A|^m\,\sqrt{Q_m(k)}, \tag{2.27}$$

where Q_m an m^{th} degree polynomial with integer coefficients. An explicit formula for Q_m is presented in Section 4.

Similarly,

$$\|\,(p-\eta)\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\,\| \;=\; \left(\frac{\hbar}{2}\right)^{1/2}\,|B|\,\sqrt{2k+1}, \tag{2.28}$$

$$\|\,(p-\eta)^2\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\,\| \;=\; \left(\frac{\hbar}{2}\right)\,|B|^2\,\sqrt{6k^2+6k+3}, \tag{2.29}$$

$$\|\,(p-\eta)^3\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\,\| \;=\; \left(\frac{\hbar}{2}\right)^{3/2}\,|B|^3\,\sqrt{20k^3+30k^2+40k+15}, \tag{2.30}$$

and

$$\|\,(p-\eta)^m\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\,\| \;=\; \left(\frac{\hbar}{2}\right)^{m/2}\,|B|^m\,\sqrt{Q_m(k)}. \tag{2.31}$$

Remark 2.7 The formulas (2.24) and (2.28) give the position and momentum uncertainties of the wave packets, respectively. The relation (2.1) can be restated as $\mathrm{Re}\,(\overline{A}\,B) \;=\; 1$, which implies $|A|\,|B| \,\geq 1$. Thus, the uncertainty product for the k^{th} state is $\hbar\,|A|\,|B|\,\left(k+\frac{1}{2}\right) \,\geq\, \hbar\,\left(k+\frac{1}{2}\right)$. When A and B are real multiples of one another and $k \,=\, 0$, the minimum uncertainty product $\hbar/2$ is attained.

We extend our exact results for quadratic Hamiltonians to approximate results for more general Hamiltonians by using this information and the following lemma.

Lemma 2.8 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

$$i\,\hbar\,\frac{\partial\psi}{\partial t}(t,\,\hbar) \;=\; H(\hbar)\,\psi(t,\,\hbar) \;+\; \zeta(t,\,\hbar), \tag{2.32}$$

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

$$\|\,\zeta(t,\,\hbar)\,\| \;\le\; \mu(t,\,\hbar).$$

Then,

$$\|\,e^{-itH(\hbar)/\hbar}\,\psi(0,\,\hbar) \;-\; \psi(t,\,\hbar)\,\| \;\le\; \hbar^{-1}\,\int_0^t\,\mu(s,\,\hbar)\,ds. \tag{2.33}$$

Proof: By the unitarity of the propagator $e^{-itH(\hbar)/\hbar}$ and the fundamental theorem of calculus, the quantity on the left-hand side of (2.33) can be estimated as follows:

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

This proves the lemma. ■

The following theorem gives leading order information for semiclassical dynamics. For $k=0$, it is essentially a restatement of Theorem 1.1 of [11].

Theorem 2.9 Suppose $V \in C^3(\mathbb{R})$ satisfies $-C_1 \le V(x) \le C_2 e^{Mx^2}$ for some C_1, C_2, and M. Let $(A(t),\, B(t),\, a(t),\, \eta(t),\, S(t))$ be a solution to the system

$$\begin{aligned} \dot{a}(t) &= \eta(t) \\ \dot{\eta}(t) &= -\, V'(a(t)) \\ \dot{A}(t) &= i\, B(t) \\ \dot{B}(t) &= i\, V''(a(t))\, A(t) \\ \dot{S}(t) &= \frac{\eta(t)^2}{2} - V(a(t)). \end{aligned} \tag{2.34}$$

Let $H(\hbar) = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2} + V(x)$. Then there exists $C(k,\, t)$, such that

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

For $t \in [0,\, T]$, fixed k, and $\hbar$ restricted to sufficiently small values, one can choose $C(k,t)$ to be any value greater than

$$\frac{1}{12}\sqrt{\frac{1}{2}(20k^3 + 30k^2 + 40k + 15)}\int_0^t |A(s)|^3\, |V'''(a(s))|\, ds. \tag{2.36}$$

Proof: Global existence and uniqueness of solutions to the system (2.34) are standard results.

We note that because V''' is uniformly continuous on any compact set, it is sufficient to prove the theorem with (2.36) replaced by

$$\frac{1}{12}\sqrt{\frac{1}{2}(20k^3 + 30k^2 + 40k + 15)}\int_0^t |A(s)|^3\, F_b(s)\, ds, \tag{2.37}$$

where

$$F_b(s) = \max_{|z-a(s)|\le b} |V'''(z)|,$$

and $b > 0$ is arbitrarily small. We also note that errors of order higher than $O(\hbar^{1/2})$ can be ignored when proving (2.35) and (2.37).

We fix a solution to the system (2.34) and let $U_\hbar(t,\, s)$ be the unitary propagator of Corollary 2.6 associated with the quadratic quantum Hamiltonian

$$H_1(t,\, \hbar) = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2} + V(a(t)) + V'(a(t))(x - a(t)) + V''(a(t))(x - a(t))^2/2.$$

The wave packet $e^{iS(t)/\hbar}\varphi_k(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, \cdot)$ satisifes

$$i\,\hbar \frac{\partial \psi}{\partial t} \;=\; H_1(t,\, \hbar)\, \psi.$$

So, by Lemma 2.8, estimate (2.35) follows from the estimate

$$\begin{aligned} &\|\, (\, H(\hbar) \,-\, H_1(t,\, \hbar)\,)\, e^{iS(t)/\hbar}\varphi_k(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, \cdot)\, \| \\ &\le\, \hbar^{3/2}\, G(t) \,+\, o(\hbar^{3/2}), \end{aligned} \tag{2.38}$$

where $C(k,\, t) \,\ge\, \displaystyle\int_0^t G(s)\, ds$. To establish (2.37), we show that (2.38) is satisfied with

$$G(t) \;=\; \frac{1}{12}\, \sqrt{\frac{1}{2}(20k^3 + 30k^2 + 40k + 15)}\, |A(t)|^3\, F_b(t). \tag{2.39}$$

To prove (2.38) with G given by (2.39), we note that our hypotheses on V and standard Taylor series estimates imply

$$\begin{aligned} &\left|\, (\, H(\hbar) \,-\, H_1(t,\, \hbar)\,)\, e^{iS(t)/\hbar}\varphi_k(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, x)\, \right| \\ &\le\, \chi_{1,b}(x,t)\, |\, (\, H(\hbar) \,-\, H_1(t,\, \hbar)\,)\, \varphi_k(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, x)\, | \\ &\qquad +\, \chi_{2,b}(x,t)\, |\, (\, H(\hbar) \,-\, H_1(t,\, \hbar)\,)\, \varphi_k(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, x)\, | \\ &\le\, \chi_{1,b}(x,t)\, \frac{1}{6} \left| V'''(z(x,t))\, (x - a(t))^3 \right|\, |\, \varphi_k(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, x)\, | \\ &\qquad +\, \chi_{2,b}(x,t)\, C_3\, e^{Mx^2}\, |\, \varphi_k(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, x)\, |\,, \end{aligned} \tag{2.40}$$

for some C_3, where $\chi_{1,b}$ is the characteristic function of the set $\{\, x \,:\, |x - a(t)| \,\le\, b\,\}$, $\chi_{2,b}(x,t) = 1 - \chi_{1,b}(x,t)$, and the $z(x,t)$ satisfies $|z(x,t) - a(t)| \le b$.

It follows from Remark 2.2 that the norm of the second term on the right hand side of (2.40) is $o(\hbar^p)$ for any p. This estimate holds uniformly for t in any compact interval. The first term on the right hand side of (2.40) is dominated by

$$\frac{1}{6}\, F_b(t)\, |x - a(t)|^3\, |\, \varphi_k(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, x)\, |\,.$$

By formula (2.26), the norm of this quantity is

$$\frac{\hbar^{3/2}}{12}\, \sqrt{\frac{1}{2}(20k^3 + 30k^2 + 40k + 15)}\, |A(t)|^3\, F_b(t),$$

which is the right hand side of (2.39).

The theorem follows. ∎

Formulas (2.8), (2.9), and (2.22) show that in the basis $\{\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,x)\,\}$, the operator $x\,-\,a$ is represented by the infinite matrix

$$\sqrt{\hbar/2}\;\begin{pmatrix} 0 & \overline{A}\sqrt{1} & 0 & 0 & 0 & 0 & \cdots \\ A\sqrt{1} & 0 & \overline{A}\sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & A\sqrt{2} & 0 & \overline{A}\sqrt{3} & 0 & 0 & \cdots \\ 0 & 0 & A\sqrt{3} & 0 & \overline{A}\sqrt{4} & 0 & \cdots \\ 0 & 0 & 0 & A\sqrt{4} & 0 & \overline{A}\sqrt{5} & \cdots \\ 0 & 0 & 0 & 0 & A\sqrt{5} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

and the operator $p\,-\,\eta$ is represented by

$$i\;\sqrt{\hbar/2}\;\begin{pmatrix} 0 & -\overline{B}\sqrt{1} & 0 & 0 & 0 & 0 & \cdots \\ B\sqrt{1} & 0 & -\overline{B}\sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & B\sqrt{2} & 0 & -\overline{B}\sqrt{3} & 0 & 0 & \cdots \\ 0 & 0 & B\sqrt{3} & 0 & -\overline{B}\sqrt{4} & 0 & \cdots \\ 0 & 0 & 0 & B\sqrt{4} & 0 & -\overline{B}\sqrt{5} & \cdots \\ 0 & 0 & 0 & 0 & B\sqrt{5} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

By a routine induction, the $k,\,j$ matrix element of $\bigl(x\,-\,a\bigr)^n$ is zero unless $n-|k-j|$ is a non-negative, even integer, and

$$\begin{aligned} \langle\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,x),\;\bigl(x\,-\,a\bigr)^m\,\varphi_j(A,\,B,\,\hbar,\,a,\,\eta,\,x)\,\rangle& \\ &= \hbar^{m/2}\,|A|^m\,\bigl(\overline{A}/A\bigr)^{(j-k)/2}\,M(k,\,m,\,j) \qquad (2.41)\\ &= \hbar^{m/2}\,A^{(m+k-j)/2}\,\bigl(\overline{A}\bigr)^{(m+j-k)/2}\,M(k,\,m,\,j), \end{aligned}$$

where

$$M(k,\,m,\,j)\;=\;\langle\,\varphi_k(1,\,1,\,1,\,0,\,0,\,x),\;x^m\,\varphi_j(1,\,1,\,1,\,0,\,0,\,x)\,\rangle$$

is the matrix element of x^m in the basis of eigenstates of the standard harmonic oscillator Hamiltonian. An explicit formula for $M(k,\,m,\,j)$ is presented in Section 4.

This result plays a central role in the following theorem that describes higher order semiclassical asymptotics. This theorem is a restatement of the main result of [13].

Theorem 2.10 Suppose $N\geq 2$, and $V\in C^{N+2}(\mathbb{R})$ satisfies $-C_1\,\leq\,V(x)\,\leq\,C_2e^{Mx^2}$ for some C_1, C_2, and M. Let $(A(t),\,B(t),\,a(t),\,\eta(t),\,S(t))$ be a solution to system (2.34), and let $H(\hbar) \;=\; -\,\dfrac{\hbar^2}{2}\,\dfrac{\partial^2}{\partial x^2} \;+\; V(x)$. Given c_k for $0 \le k \le K$, let $c_k(t,\,\hbar)$ be the unique solution to the Schrödinger type system

$$i\hbar\frac{dc_k}{dt}(t,\hbar) = \sum_{j=0}^{K+3N-3}\;\sum_{m=3}^{N+1}\,\hbar^{m/2}\,\frac{V^{(m)}(a(t))}{m!}A^{(m+k-j)/2}\;\left(\overline{A}\right)^{(m+j-k)/2}M(k,\,m,\,j)\,c_j(t,\hbar), \tag{2.42}$$

with initial conditions $c_k(0,\,\hbar) = c_k$ for $k \le K$, and $c_k(0,\,\hbar) = 0$ for $k > K$. Then for any $T > 0$, there exists C_3, such that $t \in [0,\,T]$ implies

$$\begin{aligned}\| \, e^{-itH(\hbar)/\hbar}\,\sum_{k=0}^{K}\;c_k\,\varphi_k(A(0),\,B(0),\,\hbar,\,a(0),\,\eta(0),\,\cdot) \\ -\;e^{iS(t)/\hbar}\sum_{k=0}^{K+3N-3}\;c_k(t,\,\hbar)\,\varphi_k(A(t),\,B(t),\,\hbar,\,a(t),\,\eta(t),\,\cdot)\,\| \\ \le\;C_3\,\hbar^{N/2}.\end{aligned} \tag{2.43}$$

Proof: We begin by establishing bounds on $c_k(t,\,\hbar)$. Let

$$p(k) \;=\; \begin{cases} 0 & \text{if} \quad 0 \le k \le K \\ \left\lceil \dfrac{k-K+2}{3} \right\rceil & \text{if} \quad k > K, \end{cases}$$

where $\lceil\alpha\rceil$ denotes the greatest integer greater than or equal to α.

Let $b_k(t,\,\hbar) \;=\; \hbar^{-p(k)/2}\,c_k(t,\,\hbar)$. Then

$$\frac{db_k}{dt}(t,\hbar) \;=\; \sum_{j=0}^{K+3N-3}\;\sum_{m=3}^{N+1}\;-\,i\,\hbar^{(m-p(k)+p(j)-2)/2}\,F_{k,j}(m,\,t,\,\hbar)\;b_j(t,\hbar), \tag{2.44}$$

where $F_{k,j}(m,\,t,\,\hbar)$ is uniformly bounded for $0 \le t \le T$ and $0 < \hbar \le 1$, and $F_{k,j}(m,\,t,\,\hbar) \;=\; 0$ if $|k-j| > m$. One can easily verify that

$$|\,p(k)\;-\;p(j)\,|\;\le\;\left\lceil \frac{|k-j|+2}{3} \right\rceil.$$

Thus, $m \ge 3$ and $|k-j| \le m$ imply

$$m\;-\;p(k)\;+\;p(j)\;-\;2\;\ge\;m\;-\;2\;-\;\left\lceil \frac{m+2}{3} \right\rceil\;\ge\;0.$$

This and (2.44) imply that $b_k(t,\,\hbar)$ is bounded, and hence that

$$|\,c_k(t,\,\hbar)\,| \;\leq\; C\;\hbar^{p(k)/2},$$

for $0\leq t\leq T$ and $0<\hbar\leq 1$.

We define

$$H_L(t,\,\hbar) \;=\; -\,\frac{\hbar^2}{2}\,\frac{\partial^2}{\partial x^2} \;+\; \sum_{m=0}^{L}\;V^{(m)}(a(t))\,(x-a(t))^m/m!.$$

We let $P(t,\,\hbar)$ be the orthogonal projection onto the span of
$\{\,\varphi_k(A(t),\,B(t),\,\hbar,\,a(t),\,\eta(t),\,\cdot)\,:\,0\leq k\leq K+3N-3\,\}$ and define

$$\widetilde{H}_L(t,\,\hbar) \;=\; P(t,\,\hbar)\,H_L(t,\,\hbar)\,P(t,\,\hbar).$$

The vector

$$\psi(t,\,\hbar) \;=\; e^{iS(t)/\hbar}\sum_{k=0}^{K+3N-3}\;c_k(t,\,\hbar)\,\varphi_k(A(t),\,B(t),\,\hbar,\,a(t),\,\eta(t),\,\cdot)$$

is in the range of $P(t,\,\hbar)$. For each k, $e^{iS(t)/\hbar}\phi_k(A(t),\,B(t),\,\hbar,\,a(t),\,\eta(t),\,\cdot)$ satisfies $i\,\hbar\,\dfrac{\partial\phi}{\partial t} \;=\; H_2(t,\,\hbar)\,\phi$, and the coefficients in (2.42) are obtained from the matrix elements (2.41). Thus, we see that $\psi(t,\,\hbar)$ satisfies

$$i\,\hbar\,\frac{\partial\psi}{\partial t}(t,\,\hbar) \;=\; H_{N+1}(t,\,\hbar)\,\psi(t,\,\hbar).$$

Thus,

$$\begin{aligned}\zeta(t,\,\hbar) \;&=\; i\,\hbar\frac{\partial\psi}{\partial t}(t,\,\hbar) \;-\; H(\hbar)\,\psi(t,\,\hbar)\\ &=\; \zeta_1(t,\,\hbar) \;+\; \zeta_2(t,\,\hbar),\end{aligned}$$

where

$$\zeta_1(t,\,\hbar) \;=\; (H_{N+1}(t,\,\hbar)\;-\;H(\hbar))\;\psi(t,\,\hbar),$$

and

$$\zeta_2(t,\,\hbar) \;=\; -\,(1-P(t,\,\hbar))\;\widetilde{H}_{N+1}(t,\,\hbar)\,\psi(t,\,\hbar).$$

By Lemma 2.8, we need only show that these two vectors have norms that are $O(\hbar^{(N+2)/2})$, uniformly for $t\in[0,\,T]$.

We rewrite $\zeta_1(t,\,\hbar)$ as

$$\begin{aligned}\zeta_1(t,\,\hbar,\,x) \;&=\; \left(\sum_{m=0}^{N+1} \frac{V^{(m)}(a(t))}{m!}\,(x-a(t))^m \;-\; V(x)\right)\;\psi(t,\,\hbar,\,x)\\ &=\; \frac{V^{(N+2)}(z(x,\,t))}{(N+2)!}\,(x-a(t))^{(N+2)}\;\psi(t,\,\hbar,\,x),\end{aligned} \tag{2.45}$$

where $z(x,\,t)$ lies between x and $a(t)$. We choose $\chi_{1,b}$ and $\chi_{2,b}$ exactly as in (2.40). By (2.27) and (2.45), we have

$$\|\,\chi_{1,b}(\cdot,\,t)\,\zeta_1(t,\,\hbar)\,\| \;\le\; C\,\hbar^{(N+2)/2},$$

uniformly for $t \in [0,\,T]$ and $\hbar \le 1$. As in the proof of Theorem 2.9, $\|\,\chi_{1,b}(\cdot,\,t)\,\zeta_1(t,\,\hbar)\,\|$ is of infinite order in $\hbar$.

We write $\zeta_2(t,\,\hbar)$ as

$$\zeta_2(t,\,\hbar) \;=\; \sum_{k=K+3N-2}^{K+4N-1}\;\sum_{m=3}^{N+1}\;\sum_{j=0}^{K+3N-3}\; d_{k,m,j}(t,\,\hbar)\,\varphi_k(A(t),\,B(t),\,\hbar,\,a(t),\,\eta(t),\,\cdot), \tag{2.46}$$

where

$$d_{k,m,j}(t,\,\hbar) \;=\; -\,\hbar^{m/2}\,\frac{V^{(m)}(a(t))}{m!}\,A^{(m+k-j)/2}\;\left(\overline{A}\right)^{(m+j-k)/2}\;M(k,\,m,\,j)\,c_j(t,\hbar).$$

To prove $\|\,\zeta_1(t,\,\hbar)\,\| \;\le\; C\,\hbar^{(N+2)/2}$, we need only show $|d_{k,m,j}(t,\,\hbar)| \;\le\; C\,\hbar^{(N+2)/2}$ for the values of k, m, and j that occur in (2.46). However, for $t \in [0,\,T]$, $d_{k,m,j}(t,\,\hbar)$ is a bounded function of t times $\hbar^{m/2}\,c_j(t,\hbar) \;=\; O(\hbar^{(m+p(j))/2})$. Thus, we need only show that $m+p(j) \;\ge\; N+2$ for all appropriate values of m and j.

In (2.46), non-trivial contributions occur only when $3 \,\le\, m \le\, N+1,\;\; 0 \,<\, k-j \,\le\, m$, and $k \,\ge\, K+3N-2$. The last two inequalities force $j \,\ge\, K+3N-2-m$. Then $m \,\ge\, 3$ implies

$$m\,+\,p(j) \;=\; \max\left\{m,\,m+\left[\frac{3N-m}{3}\right]\right\} \;=\; m\,+\,N\,+\,\left[-\,\frac{m}{3}\right] \;\ge\; N\,+\,2.$$

This implies the theorem. ■

We end this section by using the raising and lowering operators to show our wave packets are the same as those defined in [13]. For simplicity, we do this for $a \,=\, \eta \,=\, 0$.

By explicit calculation,

$$\mathcal{A}(A,\,B,\,\hbar,\,0,\,0)^*\,\psi(x) \;=\; -\,\overline{A}\,\sqrt{\frac{\hbar}{2}}\;\;\frac{1}{g(A,\,B,\,\hbar,\,x)}\;\;\frac{\partial}{\partial x}\,\Big(\,g(A,\,B,\,\hbar,\,x)\,\psi(x)\,\Big),$$

where

$$g(A,\,B,\,\hbar,\,x) \;=\; \exp\,\Big\{\,\overline{B}\;\overline{A}^{-1}\,x^2/(2\hbar)\,\Big\}.$$

From this we see that

$$\begin{aligned}
&\varphi_k(A,\,B,\,\hbar,\,0,\,0,\,x)\\
&\quad=\;\frac{1}{k!}\;(\,\mathcal{A}(A,\,B,\,\hbar,\,0,\,0)^*\,)^k\;\;\varphi_0(A,\,B,\,\hbar,\,0,\,0,\,x)\\
&\quad=\;\frac{1}{\sqrt{2^k\,k!}}\;\frac{1}{g(A,\,B,\,\hbar,\,x)}\;\left(\,-\,\overline{A}\,\frac{\partial}{\partial x}\,\right)^k\;(\,g(A,\,B,\,\hbar,\,x)\,\varphi_0(A,\,B,\,\hbar,\,0,\,0,\,x)\,)\,.
\end{aligned}$$

We note that

$$g(A,\,B,\,\hbar,\,x)\;\varphi_0(A,\,B,\,\hbar,\,0,\,0,\,x) \;=\; e^{-\,|A|^{-2}\,x^2/\hbar},$$

and that

$$\left(\,-\,\overline{A}\,\frac{\partial}{\partial x}\,\right)^k \;=\; A^{-k/2}\,(\overline{A})^{k/2}\;\left(\,-\,|A|\,\frac{\partial}{\partial x}\,\right)^k.$$

Thus, we have

$$\varphi_k(A,\,B,\,\hbar,\,0,\,0,\,x) \;=\; 2^{-k/2}\,(k!)^{-1/2}\;F_k(A,\,\hbar,\,x)\;\varphi_0(A,\,B,\,\hbar,\,0,\,0,\,x),$$

where

$$\begin{aligned}
F_k(A,\,\hbar,\,x) \;&=\; A^{-k/2}\,(\overline{A})^{k/2}\;e^{|A|^{-2}x^2/\hbar}\;\left(\,-\,\sqrt{\hbar}\,|A|\,\frac{\partial}{\partial x}\,\right)^k\;e^{-|A|^{-2}x^2/\hbar}\\
&=\; A^{-k/2}\,(\overline{A})^{k/2}\;H_k\left(\,\hbar^{-1/2}|A|^{-1}x\,\right).
\end{aligned}$$

Here, H_k is the k^{th} order Hermite polynomial, and we have used the standard formula

$$H_k(z) \;=\; e^{z^2}\,\left(\,-\,\frac{\partial}{\partial z}\,\right)^k\;e^{-z^2}.$$

Thus, our new definition of $\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,x)$ is equivalent to the following one that is given in [13].

Definition For $k\,=\,0,\,1,\,2,\,\ldots,$ we define

$$\begin{aligned}
\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,x) \;&=\; 2^{-k/2}\,(k!)^{-1/2}\,\pi^{-1/4}\,\hbar^{-1/4}\,A^{-(k+1)/2}\,(\overline{A})^{k/2}\\
&\quad\times\;H_k\left(\hbar^{-1/2}|A|^{-1}(x-a)\right)\;\exp\Big\{\,-\,BA^{-1}\,(x-a)^2/(2\hbar)\;+\;i\,\eta\,(x-a)/\hbar\Big\}\,.
\end{aligned}$$

Here H_k denotes the k^{th} Hermite polynomial and the choices of the square roots of A and $\overline{A}$ depend on the context.

Remark 2.11 Using the calculations above, we also see that the polynomials $F_k(A,\, \hbar,\, x)$ have a generating function, *i.e.*,

$$\sum_{k=0}^{\infty} F_k(A,\, \hbar,\, x)\, \frac{\lambda^k}{k!} \;=\; e^{-\frac{\overline{A}}{A}\,\lambda^2 + 2A^{-1}\lambda x/\sqrt{\hbar}}. \tag{(2.47)}$$

3. The Multi–Dimensional Case

The multi–dimensional case is analogous to the one–dimensional case, but one must be careful because of the transposes, conjugates, and adjoints of matrices appear in a few surprising places.

Throughout this section we assume $a \in \mathbb{R}^n$, $\eta \in \mathbb{R}^n$, and $\hbar > 0$. We also assume that A and B are $n \times n$ complex matrices that satisfy

$$A^t\, B \;-\; B^t\, A \;=\; 0, \tag{3.1}$$

$$A^*\, B \;+\; B^*\, A \;=\; 2\, I, \tag{3.2}$$

where I is the $n \times n$ identity matrix.

Conditions (3.1) and (3.2) are equivalent to the four (redundant) conditions assumed in [11, 15]. In particular, (3.2) implies that A and B are invertible because it implies

$$\langle A\, z,\, B\, z\rangle \;+\; \langle B\, z,\, A\, z\rangle \;=\; 2\, \|z\|^2,$$

where $\langle\, w,\, z\, \rangle \;=\; \sum_{j=1}^n \overline{w}_j z_j$ is the complex Euclidean inner product. If A or B had a non-trivial kernel, then by choosing $z \neq 0$ to be in the kernel, the left hand side would be zero, but right hand side would be positive. Next (3.1) implies the requirement,

$$BA^{-1} \text{ is symmetric} \quad (\,[\,\text{real symmetric} \;+\; i\,\text{real symmetric}\,]\,). \tag{3.3}$$

Furthermore, (3.2) forces

$$\left(\mathrm{Re}\, BA^{-1}\right)^{-1} \;=\; AA^*, \tag{3.4}$$

and $\mathrm{Re}\, BA^{-1}$ to be strictly positive definite.

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

$$\begin{aligned}\mathcal{A}(A,\,B,\,\hbar,\,a,\,\eta,\,v)^* &= \frac{1}{\sqrt{2\hbar}}\left[\langle\, B\,\overline{v},\,\Big(x\,-\,a\Big)\,\rangle\,-\,i\,\langle\, A\,\overline{v},\,(\,p\,-\,\eta\,)\,\rangle\right] \qquad (3.5)\\ &= \frac{1}{\sqrt{2\hbar}}\left[\sum_{j,k=1}^{n}\overline{B}_{j,k}v_k\big(x_j-a_j\big)\,-\,i\,\sum_{j,k=1}^{n}\overline{A}_{j,k}v_k\left(-i\hbar\frac{\partial}{\partial x_j}-\eta_j\right)\right],\end{aligned}$$

and

$$\begin{aligned}\mathcal{A}(A,\,B,\,\hbar,\,a,\,\eta,\,v) &= \frac{1}{\sqrt{2\hbar}}\left[\langle\,\overline{B}\,v,\,\Big(x\,-\,a\Big)\,\rangle\,+\,i\,\langle\,\overline{A}\,v,\,(\,p\,-\,\eta\,)\,\rangle\right] \qquad (3.6)\\ &= \frac{1}{\sqrt{2\hbar}}\left[\sum_{j,k=1}^{n}B_{j,k}\overline{v}_k\big(x_j-a_j\big)\,+\,i\,\sum_{j,k=1}^{n}A_{j,k}\overline{v}_k\left(-i\hbar\frac{\partial}{\partial x_j}-\eta_j\right)\right].\end{aligned}$$

By explicit calculation, we have

$$\mathcal{A}(A,B,\hbar,a,\eta,v)\;\mathcal{A}(A,B,\hbar,a,\eta,w)\;-\mathcal{A}(A,B,\hbar,a,\eta,w)\;\mathcal{A}(A,B,\hbar,a,\eta,v)\;=0, \qquad (3.7)$$

$$\mathcal{A}(A,B,\hbar,a,\eta,v)^*\mathcal{A}(A,B,\hbar,a,\eta,w)^*-\mathcal{A}(A,B,\hbar,a,\eta,w)^*\mathcal{A}(A,B,\hbar,a,\eta,v)^*=0, \qquad (3.8)$$

$$\mathcal{A}(A,B,\hbar,a,\eta,v)\;\mathcal{A}(A,B,\hbar,a,\eta,w)^*-\mathcal{A}(A,B,\hbar,a,\eta,w)^*\mathcal{A}(A,B,\hbar,a,\eta,v)\;=\langle v,\,w\rangle. \qquad (3.9)$$

At this point, one can choose any orthonormal basis of $\mathbb{R}^n$. For convenience, we choose the standard basis $\{\,e_j\,\}$, and define

$$\begin{aligned}\mathcal{A}_j(A,\,B,\,\hbar,\,a,\,\eta)^* &= \mathcal{A}(A,\,B,\,\hbar,\,a,\,\eta,\,e_j)^*\\ \mathcal{A}_j(A,\,B,\,\hbar,\,a,\,\eta) &= \mathcal{A}(A,\,B,\,\hbar,\,a,\,\eta,\,e_j),\;\;.\end{aligned}$$

We let $\mathcal{A}(A,\,B,\,\hbar,\,a,\,\eta)^*$ and $\mathcal{A}(A,\,B,\,\hbar,\,a,\,\eta)$ denote the formal vectors whose components are the n raising and lowering operators, respectively. We then have

$$\mathcal{A}(A,\,B,\,\hbar,\,a,\,\eta)^* \;=\; B^*\,(x-a)\;-\;i\,A^*\,(p-\eta) \qquad (3.10)$$

$$\mathcal{A}(A,\,B,\,\hbar,\,a,\,\eta) \;=\; B^t\,(x-a)\;+\;i\,A^t\,(p-\eta) \qquad (3.11)$$

For simplicity, we adopt standard multi-index notation. A multi-index $k = (k_1,\,k_2,\,\ldots,\,k_n)$ is an n–tuple of non-negative integers. We define the order of k to be $|k| \;=\; \sum_{j=1}^{n} k_j$ and the factorial of k to be $k! = (k_1!)(k_2!)\dots(k_n!)$. We let $D^k = \frac{\partial^{|k|}}{(\partial x_1)^{k_1}(\partial x_2)^{k_2}\dots(\partial x_n)^{k_n}}$, and $x^k = x_1^{k_1}x_2^{k_2}\dots x_n^{k_n}$.

Definition By solving the trivial system of first order linear partial differential equations,

$$\mathcal{A}(A,\,B,\,\hbar,\,a,\,\eta)\,\varphi_0(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\;=\;0,\tag{3.12}$$

we see that the intersection of the kernels of the lowering operators is a one-dimensional subspace. Modulo a plus or minus sign, we fix the phase and normalization of the solution to (3.12) by the formula

$$\begin{aligned}&\varphi_0(A,\,B,\,\hbar,\,a,\,\eta,\,x)\\&\quad=\pi^{-n/4}\hbar^{-n/4}(\det(A))^{-1/2}\exp\left\{-\langle(x-a),\,BA^{-1}(x-a)\rangle/(2\hbar)+i\,\langle\eta,\,(x-a)\rangle/\hbar\right\}.\end{aligned}\tag{3.13}$$

Then for any multi-index k, we define

$$\begin{aligned}&\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\\&\qquad=\frac{1}{\sqrt{k!}}\,\left(\mathcal{A}_1(A,\,B,\,\hbar,\,a,\,\eta)^*\right)^{k_1}\left(\mathcal{A}_2(A,\,B,\,\hbar,\,a,\,\eta)^*\right)^{k_2}\,\dots\\&\qquad\qquad\left(\mathcal{A}_n(A,\,B,\,\hbar,\,a,\,\eta)^*\right)^{k_n}\;\varphi_0(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot).\end{aligned}\tag{3.14}$$

Remark 3.1 Formulas (3.12) and (3.14) define all the functions $\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)$, modulo a single numerical phase. Our explicit formula (3.13) reduces the ambiguity to the choice of the sign of $A^{-1/2}$. The particular choice of that sign depends on the context.

Remark 3.2 It is easy to see that $\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,x)$ is a $|k|^{\text{th}}$ degree polynomial in the components of $\frac{x-a}{\sqrt{\hbar}}$ times $\varphi_0(A,\,B,\,\hbar,\,a,\,\eta,\,x)$. The definition of $\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,x)$ in [15] involves a recursive construction of these polynomials that is lengthy, unituitive, and involves the polar decomposition of the matrix A.

Theorem 3.3 The functions $\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)$, form an orthonormal basis of $L^2(\mathbb{R}^n)$. They satisfy

$$\mathcal{A}_j(A,\,B,\,\hbar,\,a,\,\eta)\;\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\;=\;\sqrt{k_j}\;\varphi_{k'}(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot),\tag{3.15}$$

where $k' = (k_1, \ldots, k_{j-1}, k_j - 1, k_{j+1}, \ldots, k_n)$,

$$\mathcal{A}_j(A,\, B,\, \hbar,\, a,\, \eta)^* \, \varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot) \;=\; \sqrt{k_j + 1}\; \varphi_{k''}(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot), \tag{3.16}$$

where $k'' = (k_1, \ldots, k_{j-1}, k_j + 1, k_{j+1}, \ldots, k_n)$,

$$\mathcal{A}_j(A,\, B,\, \hbar,\, a,\, \eta)^* \mathcal{A}_j(A,\, B,\, \hbar,\, a,\, \eta)\; \varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot) \;=\; k_j\; \varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot), \tag{3.17}$$

$$\mathcal{A}_j(A,\, B,\, \hbar,\, a,\, \eta) \mathcal{A}_j(A,\, B,\, \hbar,\, a,\, \eta)^*\; \varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot) \;=\; (k_j + 1)\; \varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot). \tag{3.18}$$

Proof: We simply mimic the proof of Theorem 2.3 and do several inductions on $|k|$. ■

We define the scaled Fourier transform by

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

Then the analogs of (2.12) and (2.13) hold for each $\mathcal{A}_j$ and $\mathcal{A}_j^*$. Furthermore, for any multi-index k, we have the following analog of (2.15):

$$(\mathcal{F}_\hbar\, \varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, \cdot))(\xi) \;=\; (-i)^{|k|}\; e^{-i\langle a,\, \eta\rangle/\hbar}\; \varphi_k(B,\, A,\, \hbar,\, \eta,\, -a,\, \xi). \tag{3.19}$$

This result is Lemma 2.2 of [15]. The old proof of this beautiful result that is presented in [15] is an induction in $|k|$ that contains a horrible, unintuitive calculation.

We now turn to the n–dimensional analogs of the results of Section 2 for time–dependent quadratic Hamiltonians. Suppose $\alpha(\cdot)$, $\beta(\cdot)$, and $\gamma(\cdot)$ are continuous, real, $n \times n$ matrix–valued funtions; $\delta(\cdot)$ and $\epsilon(\cdot)$ are continuous, $\mathbb{R}^n$–valued functions; and $\zeta(\cdot)$ is continuous and real valued. Assume $\alpha(t)$ and $\gamma(t)$ are symmetric for each t, and let $\beta^t(t)$ denote the transpose of $\beta(t)$. We consider the classical Hamiltonian

$$H(x,\, p,\, t) \;=\; \frac{1}{2} \begin{pmatrix} p \\ x \end{pmatrix} \cdot \begin{pmatrix} \alpha(t) & \beta(t) \\ \beta^t(t) & \gamma(t) \end{pmatrix} \begin{pmatrix} p \\ x \end{pmatrix} \;+ \langle \delta(t),\, p \rangle \;+\; \langle \epsilon(t),\, x \rangle \;+\; \zeta(t).$$

Given any initial conditions $(A(0),\, B(0),\, a(0),\, \eta(0),\, S(0))$, there exists a unique solution $(A(t),\, B(t),\, a(t),\, \eta(t),\, S(t))$ to the system

$$\begin{aligned}
\dot{a}(t) \;&= \beta(t)\, a(t) \;+\; \alpha(t)\, \eta(t) \;+\; \delta(t) \\
\dot{\eta}(t) \;&=\; -\,\gamma(t)\, a(t) \;-\; \beta^t(t) \eta(t) \;-\; \epsilon(t) \\
\dot{A}(t) \;&= \beta(t)\, A(t) \;+\; i\, \alpha(t)\, B(t) \\
\dot{B}(t) \;&= i\, \gamma(t)\, A(t) \;-\; \beta^t(t)\, B(t) \\
\dot{S}(t) \;&= \alpha(t)\, \frac{\eta(t)^2}{2} \;-\; \gamma(t)\, \frac{a(t)^2}{2} \;-\; \epsilon(t)\, a(t) \;-\; \zeta(t).
\end{aligned} \tag{3.20}$$

The solutions to the equations for A and B can be written in terms of the derivative of the phase space flow associated with a and η. Explicitly, we have

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

One proves these formulas by observing that the left and right hand sides of the equations satisfy the same differential equations and same initial conditions.

For the corresponding quantum mechanical system, we have the following:

Theorem 3.4 Let $\alpha(\cdot)$, $\beta(\cdot)$, $\gamma(\cdot)$, $\delta(\cdot)$, $\epsilon(\cdot)$, and $\zeta(\cdot)$ be as above. Let $(A(\cdot),\, B(\cdot),\, a(\cdot),\, \eta(\cdot),\, S(\cdot))$ be any solution to the system (3.20). Then, for every k,

$$\psi(\hbar,\, t) \;=\; e^{iS(t)/\hbar}\, \varphi_k(A(t),\, B(t),\, \hbar,\, a(t),\, \eta(t),\, \cdot) \tag{3.21}$$

satisfies the Schrödinger equation

$$i\,\hbar\, \frac{\partial \psi}{\partial t} \;=\; H(t)\, \psi, \tag{3.22}$$

for the time–dependent quantum Hamiltonian

$$\begin{aligned} H(t) \;=\; &-\frac{\hbar^2}{2} \sum_{i,j} \alpha_{i,j}(t) \frac{\partial^2}{\partial x_i \partial x_j} \;-\; \frac{i\hbar}{2} \sum_{i,j} \beta_{i,j}(t) \left\{ x_j\, \frac{\partial}{\partial x_i} \;+\; \frac{\partial}{\partial x_i}\, x_j \right\} \\ &+\; \frac{1}{2} \sum_{i,j} \gamma_{i,j}(t)\, x_i x_j \;-\; i\hbar \sum_i \delta_i(t)\, \frac{\partial}{\partial x_i} \;+\; \sum_i \epsilon_i(t)\, x_i \;+\; \zeta(t). \end{aligned} \tag{3.23}$$

Furthermore, the analog of Corollary 2.6 holds for this Hamiltonian.

Proof: We simply mimic the proofs of Theorem 2.5 and Corollary 2.6. ∎

From conditions (3.3) and (3.4), we see that AA^* is a real symmetric matrix. Thus,

$$AA^* \;=\; (AA^*)^t \;=\; \overline{A}A^t \tag{3.24}$$

This, (3.1) and (3.2) imply

$$\begin{aligned} A\,B^* \;+\; \overline{A}\,B^t &= A\,B^* \;+\; \overline{A}\,B^t\,A\,A^{-1} \\ &= A\,B^* \;+\; \overline{A}\,A^t\,B\,A^{-1} \\ &= A\,B^* \;+\; A\,A^*\,B\,A^{-1} \\ &= A\,(B^*\,A \;+\; A^*\,B)\,A^{-1} \\ &= 2\,I. \end{aligned} \tag{3.25}$$

Similarly, we have

$$BB^* \;=\; (BB^*)^t \;=\; \overline{B}B^t \tag{3.26}$$

and

$$\overline{B}\,A^t \,+\, B\,A^* \;=\; 2\,I. \tag{3.27}$$

Using formulas (3.10), (3.11), and (3.24)–(3.27), we then see that, as operators on $\mathcal{S}$, we have

$$x \,-\, a \;=\; \sqrt{\frac{\hbar}{2}}\,\left(A\,\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)^* \,+\, \overline{A}\,\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)\right), \tag{3.28}$$

and

$$p \,-\, \eta \;=\; i\sqrt{\frac{\hbar}{2}}\,\left(B\,\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)^* \,-\, \overline{B}\,\mathcal{A}(A,\,B,\,\hbar,\,a,\eta)\right). \tag{3.29}$$

From these formulas, one can compute n–dimensional analogs of (2.24)–(2.31), but they are complicated. However, one easily sees that for any multi-index k,

$$\|(x_j - a_j)\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\| \;=\; \left(\frac{\hbar}{2}\right)^{1/2}\,\left(\sum_{l=1}^{n}\,|A_{j,l}|^2\,(2k_l+1)\right)^{1/2},$$

and for any multi-indices m and k,

$$\|(x-a)^m\,\varphi_k(A,\,B,\,\hbar,\,a,\,\eta,\,\cdot)\| \;=\; O(\hbar^{|m|/2}). \tag{3.30}$$

To state the analogs of Theorems 2.9 and 2.10, we let $V^{(1)}$ denote the gradient of V, $V^{(2)}$ denote the Hessian matrix of second partial derivatives, etc.

Theorem 3.5 Suppose $V \in C^3(\mathbb{R}^n)$ satisfies $-\,C_1 \,\le\, V(x) \,\le C_2\,e^{Mx^2}$ for some C_1, C_2, and M. Let $(A(t),\,B(t),\,a(t),\,\eta(t),\,S(t))$ be a solution to the system

$$\begin{aligned}
\dot{a}(t) \;&=\eta(t)\\
\dot{\eta}(t) \;&=\; -\,V^{(1)}(a(t))\\
\dot{A}(t) \;&=i\,B(t)\\
\dot{B}(t) \;&=i\,V^{(2)}(a(t))\,A(t)\\
\dot{S}(t) \;&=\; \frac{\eta(t)^2}{2} \,-\, V(a(t)).
\end{aligned} \tag{3.31}$$

Let $H(\hbar) \;=\; -\,\dfrac{\hbar^2}{2}\,\Delta \,+\, V(x)$. Then there exists $C(k,\,t)$, such that

$$\begin{aligned}
&\|\,e^{-itH(\hbar)/\hbar}\,\varphi_k(A(0),\,B(0),\,\hbar,\,a(0),\,\eta(0),\,\cdot) \;-\; e^{iS(t)/\hbar}\varphi_k(A(t),\,B(t),\,\hbar,\,a(t),\,\eta(t),\,\cdot)\,\|\\
&\le\; C(k,\,t)\,\hbar^{1/2}.
\end{aligned} \tag{3.32}$$

Proof: We simply mimic the proof of Theorem 2.9, using (3.30) for $|m| = 3$ in place of (2.26), without bothering to keep track of the constant $C(k,\,t)$. One could estimate the constant, but the analog of (2.36) would be complicated. $\blacksquare$

The higher order result is the following:

Theorem 3.6 Suppose $N \geq 2$, and $V \in C^{N+2}(\mathbb{R}^n)$ satisfies $-C_1 \leq V(x) \leq C_2 e^{Mx^2}$ for some C_1, C_2, and M. Let $(A(t),\,B(t),\,a(t),\,\eta(t),\,S(t))$ be a solution to system (3.41), and let $H(\hbar) = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2} + V(x)$. Given c_k for $|k| \leq K$, let $c_k(t,\,\hbar)$ be the unique solution to a Schrödinger type system

$$i\,\hbar\,\frac{dc_k}{dt}(t,\hbar) \;=\; \sum_{|j|\leq K+3N-3}\;\sum_{3\leq|m|\leq N+1} \hbar^{|m|/2}\,\frac{[D^mV](a(t))}{m!}\,b_{k,m,j}(A(t))\,c_j(t,\hbar), \qquad (3.33)$$

with initial conditions $c_k(0,\,\hbar) = c_k$ for $|k| \leq K$, and $c_k(0,\,\hbar) = 0$ for $|k| > K$. (The quantity $b_{k,m,j}(A(t))$ depends continuously on $A(t)$.) Then for any $T > 0$, there exists C_3, such that $t \in [0,\,T]$ implies

$$\begin{aligned}\|\, e^{-itH(\hbar)/\hbar} \sum_{|k|\leq K} & c_k\,\varphi_k(A(0),\,B(0),\,\hbar,\,a(0),\,\eta(0),\,\cdot) \\ & -\; e^{iS(t)/\hbar} \sum_{|k|\leq K+3N-3} c_k(t,\,\hbar)\,\varphi_k(A(t),\,B(t),\,\hbar,\,a(t),\,\eta(t),\,\cdot)\,\| \\ & \leq\; C_3\,\hbar^{N/2}. \qquad (3.34)\end{aligned}$$

Proof: We simply mimic the proof of Theorem 2.10. The quantity $b_{k,m,j}(A(t))$ is the k,j matrix element of $(x-a)^m$ in the basis of $\varphi_k(A(t),\,B(t),\,\hbar,\,a(t),\,\eta(t),\,\cdot)$. $\blacksquare$

4. Matrix Elements of $(x-a)^m$ in One Dimension

In this section we present fairly explicit formulas for the quantity

$$M(k,\,m,\,j) \;=\; \langle\, \varphi_k(1,\,1,\,1,\,0,\,0,\,x),\; x^m\; \varphi_j(1,\,1,\,1,\,0,\,0,\,x)\,\rangle$$

that appears in (2.41). Although we believe these formulas must be known, we are unaware of specific references.

Theorem 4.1 The quantity $M(k, m, j)$ is non-zero only if $m - |k-j|$ is even and non-negative. The even order diagonal matrix elements are

$$M(k, m, k) = 2^{-m/2} \quad 1\cdot 3\cdot 5\cdots (m-1) \quad \sum_{p=0}^{\min\{m/2, k\}} 2^p \binom{m/2}{p} \binom{k}{p}, \tag{4.1}$$

where $\binom{a}{b}$ denotes the standard binomial coefficient.

More generally, when m and $|j-k|$ are even, let $\alpha = m/2$, $\beta = |j-k|/2$, and $\gamma = \min\{j, k\}$. Then

$$M(k, m, j) = 2^{\beta-\alpha} \quad 1\cdot 3\cdot 5\cdots(2\alpha-1) \quad \left(\frac{(\gamma+2\beta)!}{\gamma!}\right)^{1/2}$$
$$\times \quad \frac{\alpha!}{(\alpha+\beta)!} \quad \sum_{p=0}^{\min\{\alpha-\beta, \gamma\}} 2^p \binom{\gamma}{p} \binom{\alpha+\beta}{p+2\beta}. \tag{4.2}$$

When m and $|j-k|$ are odd, let $\alpha = (m-1)/2$, $\beta = (|j-k|+1)/2$, and $\gamma = \min\{j, k\}$. Then

$$M(k, m, j) = 2^{\beta-\alpha-3/2} \quad 1\cdot 3\cdot 5\cdots(2\alpha+1) \quad \left(\frac{(\gamma+2\beta-1)!}{\gamma!}\right)^{1/2}$$
$$\times \quad \frac{\alpha!}{(\alpha+\beta)!} \quad \sum_{p=0}^{\min\{\alpha-\beta+1, \gamma\}} 2^p \binom{\gamma}{p} \binom{\alpha+\beta}{p+2\beta-1}. \tag{4.3}$$

Proof: For $A = \hbar = 1$, the generating function (2.47) is well known in the form

$$\sum_{k=0}^{\infty} H_k(x)\, \frac{t^k}{k!} = e^{-t^2+2tx}.$$

It follows that

$$\begin{aligned}
&\sum_{j,k=0}^{\infty} 2^{(j+k)/2}\, (j!)^{1/2}\, (k!)^{1/2}\, \pi^{1/2}\, M(k, m, j)\, \frac{t^j\, s^k}{j!\, k!} \\
&= \int_{\mathbb{R}} e^{-s^2+2sx}\, x^m\, e^{-t^2+2tx}\, dx \\
&= 2^{2st} \int_{\mathbb{R}} e^{-(x-s-t)^2}\, x^m\, dx \\
&= \sum_{n=0}^{\infty} \frac{2^n s^n t^n}{n!} \int_{\mathbb{R}} (x+s+t)^m\, e^{-x^2}\, dx.
\end{aligned} \tag{4.4}$$

We now assume that m is even. The proof when m is odd is similar. When m is even, explicit evaluation of the last integral in (4.4) shows that the quantity (4.4) equals

$$\sum_{n=0}^{\infty} \frac{2^n s^n t^n}{n!} \sum_{\substack{l=0 \\ l \text{ even}}}^{m} \binom{m}{l} (s+t)^l \frac{1 \cdot 3 \cdot 5 \cdots (m-l-1)}{2^{(m-l)/2}} \pi^{1/2}. \tag{4.5}$$

Thus, by equating like powers of t and s in (4.4) and (4.5), we obtain

$$M(k,\, m,\, j) \;=\; 2^{-(j+k)/2} (j!)^{1/2} (k!)^{1/2}$$
$$\times \sum_{\substack{l=|j-k| \\ l \text{ even}}}^{\min\{k+j,\, m\}} \; \sum_{n=\max\{k-l,\, j-l\}}^{\min\{j,\, k\}} \frac{2^n}{n!} \binom{m}{l} \binom{l}{k-n} \frac{1 \cdot 3 \cdot 5 \cdots (m-l-1)}{2^{(m-l)/2}} \delta_{k+j,\, 2n+l}.$$

The limits on the sums and the Kronecker delta are generated by the conspiracy of trivial relations: $0 \le n$, $n \le j \le l+n$, $n \le k \le l+n$, $0 \le l \le m$, l even, and the condition $j+k = 2n+l$ which is the sum of the exponents of t and s. We note that $j-k$ must be even and that our expression for $M(k,\, m,\, j)$ is symmetric in j and k because $\binom{l}{k-n} = \binom{l}{j-n}$.

By exploiting the Kronecker delta, and using $q = l/2$, $\alpha = m/2$, $\beta = |j-k|/2$, and $\gamma = \min\{j,\, k\}$, we obtain

$$M(k,\, m,\, j) \;=\; 2^{-(j+k)/2} (j!)^{1/2} (k!)^{1/2}$$
$$\times \sum_{q=\beta}^{\min\{\alpha,\, (j+k)/2\}} \frac{2^{(j+k-2q)/2}}{((k+j-2q)/2)!} \binom{m}{2q} \binom{2q}{q-\beta} \frac{1 \cdot 3 \cdot 5 \cdots (m-2q-1)}{2^{(m-2q)/2}}.$$

We rewrite this expression as

$$\begin{aligned}
&M(k,\, m,\, j) \\
&= \; 2^{-\alpha} (j!)^{1/2} (k!)^{1/2} \\
&\quad \times \sum_{q=\beta}^{\min\{\alpha,\, (j+k)/2\}} \frac{1}{\left(\frac{j+k}{2} - q\right)!} \frac{(2\alpha)!}{(2q)!\, (2(\alpha-q))!} \frac{(2q)!}{(q-\beta)!\, (q+\beta)!} 1 \cdot 3 \cdot 5 \cdots (2(\alpha-q)-1) \\
&= \; 2^{-\alpha} (j!)^{1/2} (k!)^{1/2} \sum_{q=\beta}^{\min\{\alpha,\, (j+k)/2\}} \frac{1}{\left(\frac{j+k}{2} - q\right)!} \frac{(2\alpha)!}{2 \cdot 4 \cdot 6 \cdots (2(\alpha-q))} \frac{1}{(q-\beta)!\, (q+\beta)!} \\
&= \; 2^{-2\alpha} (j!)^{1/2} (k!)^{1/2} \sum_{q=\beta}^{\min\{\alpha,\, (j+k)/2\}} \frac{2^q}{\left(\frac{j+k}{2} - q\right)!} \frac{(2\alpha)!}{(\alpha-q)!} \frac{1}{(q-\beta)!\, (q+\beta)!}.
\end{aligned}$$

Due to the symmetry in j and k, we may assume without loss that $j \geq k$. We can then rewrite this expression as

$$
\begin{aligned}
& M(k,\, m,\, j) \\
&= 2^{-2\alpha} \left(\frac{j!}{k!}\right)^{1/2} \sum_{q=\beta}^{\min\{\alpha,\,(j+k)/2\}} \frac{2^q}{\left(\frac{j+k}{2} - q\right)!} \, \frac{(2\alpha)!}{(\alpha - q)!} \, \frac{k!}{(q-\beta)!\,(q+\beta)!} \\
&= 2^{-2\alpha} \left(\frac{j!}{k!}\right)^{1/2} \sum_{q=\beta}^{\min\{\alpha,\,(j+k)/2\}} 2^q \binom{k}{q-\beta} \frac{(2\alpha)!}{(\alpha - q)!\,(q+\beta)!} \\
&= 2^{-2\alpha} \left(\frac{j!}{k!}\right)^{1/2} \sum_{q=\beta}^{\min\{\alpha,\,(j+k)/2\}} 2^q \binom{k}{q-\beta} \binom{\alpha+\beta}{q+\beta} \frac{(2\alpha)!}{(\alpha+\beta)!}.
\end{aligned}
$$

We now replace q by $p = q - \beta$ to rewrite this as

$$
\begin{aligned}
& M(k,\, m,\, j) \\
&= 2^{-2\alpha} \, \frac{(2\alpha)!}{(\alpha+\beta)!} \left(\frac{j!}{k!}\right)^{1/2} \sum_{p=0}^{\min\{\alpha-\beta,\, k\}} 2^{p+\beta} \binom{k}{p} \binom{\alpha+\beta}{p+2\beta} \\
&= 2^{\beta-2\alpha} \, (\alpha+\beta+1)\cdot(\alpha+\beta+2)\cdots(2\alpha) \left(\frac{j!}{k!}\right)^{1/2} \sum_{p=0}^{\min\{\alpha-\beta,\, k\}} 2^{p} \binom{k}{p} \binom{\alpha+\beta}{p+2\beta} \\
&= 2^{\beta-\alpha} \, 1\cdot 3\cdot 5\cdots(2\alpha-1) \, \frac{\alpha!}{(\alpha+\beta)!} \left(\frac{j!}{k!}\right)^{1/2} \sum_{p=0}^{\min\{\alpha-\beta,\, k\}} 2^{p} \binom{k}{p} \binom{\alpha+\beta}{p+2\beta}.
\end{aligned}
$$

Our assumption $j \geq k$ implies $k = \gamma$ and $j = \gamma + 2\beta$, so this expression is equivalent to (4.2).

The calculations for odd m are similar. ∎

Corollary 4.2 The polynomial $Q_m(k)$ in (2.27) and (2.31) is

$$
Q_m(k) \;=\; 1\cdot 3\cdot 5\cdots(2m-1) \sum_{p=0}^{\min\{m,\,k\}} 2^p \binom{m}{p} \binom{k}{p}.
$$

Proof: This is an immediate consequence of (4.1), since $Q_m(k) \;=\; 2^m\, M(k,\, 2m,\, k)$. ∎

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