Bohr–Sommerfeld Quantization Rules in the Semiclassical Limit

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Abstract

We study one-dimensional quantum mechanical systems in the semiclassical limit. We construct a lowest order quasimode $\psi(\hbar)$ for the Hamiltonian $H(\hbar)$ when the energy E and Planck's constant $\hbar$ satisfy the appropriate Bohr-Sommerfeld conditions. This means that $\psi(\hbar)$ is an approximate solution of the Schrödinger equation in the sense that

$$\|[H(\hbar) - E]\,\psi(\hbar)\| \leq C\hbar^{3/2}\,\|\psi(\hbar)\|\,.$$

It follows that $H(\hbar)$ has some spectrum within a distance $C\hbar^{3/2}$ of E. Although the result has a long history, our time-dependent construction technique is novel and elementary.

1 Introduction

In this paper we construct approximate eigenfunctions for the one–dimensional, time–independent Schrödinger equation in the semiclassical limit. The history of such constructions is as rich as that of the Schrödinger equation itself, and many of the diverse methods for producing approximate eigenfunctions have come to be labelled “quasimode” constructions. For a given potential $V(x)$ and the associated Schrödinger operator $H(\hbar) = -\frac{\hbar^2}{2}\frac{d^2}{dx^2} + V(x)$, we seek a *quasi–energy* $E(\hbar)$ in $\mathbb{R}$ and a *quasimode* $\Psi(\hbar, x)$ in $L^2(\mathbb{R}, dx)$ that satisfy $\|\Psi(\hbar, \cdot)\|_{L^2(\mathbb{R})} = O(1)$ as $\hbar \searrow 0$ and

$$\|[H(\hbar) - E(\hbar)]\, \Psi(\hbar, \cdot)\|_{L^2(\mathbb{R})} \le C\hbar^\lambda \tag{1}$$

for $\lambda > 1$ and some sequence of positive values of $\hbar$ converging to zero. This implies that $H(\hbar)$ has spectrum in the interval $[E(\hbar) - C\hbar^\lambda,\, E(\hbar) - C\hbar^\lambda]$. Under the hypotheses we assume, the spacing between eigenvalues of $H(\hbar)$ is $O(\hbar)$, so our construction yields non-trivial information.

We present a novel quasimode construction based on time–dependent methods. The Bohr–Sommerfeld quantization rules arise as a sufficient condition under which our approximation holds. Our techniques require little more than some functional analysis, a little ODE theory, and some L^2 estimates. The construction of quasimodes using coherent states has been studied by others (see [10], [3], [8], and the references therein). Some historical comments and multidimensional results can be found in [13] and [11]. We note that assumptions made in some papers, such as [13] and [11], are never satisfied by non–trivial one–dimensional systems.

Near the completion of this work we learned of the unpublished doctoral thesis of Khuat-Duy [9] which contains ideas similar to those underlying our proof, though the techniques and details of the presentation are different. We thank Professors Paul and Uribe for bringing this result to our attention.

The basic idea of this paper is to construct quasimodes of the form

$$\Psi(\hbar, x) = C(\pi\hbar)^{-1/4} \int_0^{\tau(E)} e^{it(E + \frac{\pi\hbar}{\tau(E)})/\hbar} e^{iS(t)/\hbar} \varphi_0(A(t), B(t), \hbar, a(t), \eta(t), x)\, dt, \tag{2}$$

where E satisfies the Bohr–Sommerfeld conditions. The quantities $A(t)$, $B(t)$, $a(t)$, $\eta(t)$, and $S(t)$ are determined by classical mechanics, and

$$e^{iS(t)/\hbar} \varphi_0(A(t), B(t), \hbar, a(t), \eta(t), x)$$

is an approximate solution to a time–dependent Schrödinger equation that is defined below. The Bohr–Sommerfeld conditions arise in a simple, intuitive fashion as conditions on the phase of the time–dependent wave function as the system propagates around a classical periodic orbit.

1.1 Some notation and definitions

We handle a rather large class of potentials. Our assumptions on the potential $V(x)$ are:

(V1) $V \in C^5(\mathbb{R})$,

(V2) V is bounded from below by a constant,

(V3) $|V(x)| \leq Ce^{Mx^2}$ for some constants C and M,

(V4) $V_{\pm} = \lim_{x \to \pm\infty} V(x) \in \mathbb{R} \cup \{\infty\}$.

Under assumptions (V1 - V2) the Hamiltonian $H(\hbar)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}) \subset L^2(\mathbb{R})$. The degree of smoothness in (V1) and the growth condition in (V3) facilitate some estimates that arise in our proof. Assumption (V4) serves to simplify the spectral information we can extract from the quasimodes. We restrict ourselves to quasi–energies below $E_{\max} = \min\{V_-,\ V_+\}$ so our quasi–energies correspond to discrete eigenvalues of finite multiplicity.

We assume (V1 - V4) for the remainder of this paper. These assumptions are not optimal: the degree of smoothness in (V1) can be relaxed to, say, $V \in C^4(\mathbb{R})$ with $V^{(4)}$ uniformly Lipschitz; the growth condition in (V3) could be avoided by introducing "cutoffs"; and (V4) could at least be generalized (*e.g.*, by using the limit superior or inferior).

Crucial to our proof is the semiclassical time evolution of a class of Gaussian states [5] [6]. Given complex numbers A and B satisfying

$$\bar{A}B + \bar{B}A = 2, \tag{3}$$

real numbers a and η, and $\hbar > 0$ we define

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

We explicitly define the branch of the square root in this definition when necessary. The function φ_0 is normalized in the sense that it has L^2 norm (hereafter denoted by $\|\cdot\|$) equal to one.

We write $H(q,p)$ for the classical Hamiltonian

$$H(q,p) = \frac{1}{2}p^2 + V(q),$$

$H(\hbar)$ for the quantum Hamiltonian

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

and use the symbol H alone when the context is clear. For $E < E_{\text{max}}$, let $\gamma(E)$ denote a single connected component of the energy surface (actually a curve)

$$\Gamma(E) = \{(q,p) \in \mathbb{R}^2 : H(q,p) = E\}.$$

We call the trajectory $\gamma(E)$ *regular* if its projection onto the spatial component q avoids the top of a potential barrier, *i.e.*, if

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

are distinct adjacent roots of $V(q) = E$ with $V'(q_-) < 0$ and $V'(q_+) > 0$. Under such conditions, it is well known (see, *e.g.*, [4]) that the classical motion in phase space is periodic with a positive minimal period τ. The period τ depends on the initial conditions only through the energy. For a regular trajectory $\gamma(E)$ we define the "action function" I by

$$I(E) = \oint_{\gamma(E)} p\, dq.$$

Geometrically, $I(E)$ is the phase space area enclosed by the trajectory $\gamma(E)$. This function is well-defined, and implicit function arguments show that, in a neighborhood of a regular trajectory, it is as smooth in E as V is in x. It is straightforward to show that the period τ of the motion confined to $\gamma(E)$ is

$$\tau(E) = \frac{\partial}{\partial E} I(E).$$

1.2 The results

We now state our main results. We assume V satisfies assumptions (V1 - V4) and that $\gamma(E)$ is a regular trajectory. Next, we determine time-dependent quantities $a(t)$, $\eta(t)$, $A(t)$, $B(t)$, and $S(t)$ from classical mechanics. When the Bohr–Sommerfeld condition

$$I(E) = \oint_{\gamma(E)} p\, dq = 2\pi\hbar n, \;\; n \in \mathbb{Z}^+$$

is satisfied, $\Psi(\hbar, x)$ defined by (2) is a quasimode in the sense that it satisfies

$$\left\| \left[H(\hbar) - \left(E + \frac{\pi\hbar}{\tau(E)} \right) \right] \Psi(\hbar, \cdot) \right\| = O(\hbar^{3/2}).$$

The precise statement is the following:

Theorem 1 *Suppose V satisfies assumptions (V1 - V4), and $E < E_{\max}$. Suppose $\gamma(E)$ is a regular trajectory, and define $\alpha(E) = \dfrac{\tau'(E)}{2\tau(E)}$. Let A_0 and B_0 be complex numbers that satisfy (3), $(a_0, \eta_0) \in \gamma(E)$, and let $a(t)$, $\eta(t)$, $A(t)$, $B(t)$, and $S(t)$ be given by the unique solution of the system of ordinary differential equations*

$$\begin{aligned}
\dot{a}(t) &= \eta(t) && (5)\\
\dot{\eta}(t) &= -V'(a(t)) && (6)\\
\dot{A}(t) &= iB(t) + 2\alpha(E)\eta(t)\,(V'(a(t))A(t) + i\eta(t)B(t)) && (7)\\
\dot{B}(t) &= iV''(a(t))A(t) + 2i\alpha(E)V'(a(t))\,(V'(a(t))A(t) + i\eta(t)B(t)) && (8)\\
\dot{S}(t) &= \frac{1}{2}\,\eta(t)^2 - V(a(t)) && (9)
\end{aligned}$$

subject to the initial conditions

$$(a(0), \eta(0), A(0), B(0), S(0)) = (a_0, \eta_0, A_0, B_0, 0)\,.$$

Then

$$I(E) = E\,\tau(E) + S(\tau(E)). \tag{10}$$

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

$$I(E) = 2\pi\hbar n,\ \ n \in \mathbb{Z}^+ \tag{11}$$

and define

$$\begin{aligned}
\Psi(\hbar, x) &= (\pi\hbar)^{-1/4}\sqrt{\frac{|\theta|}{2\tau(E)}}\int_0^{\tau(E)} e^{it(E+\frac{\pi\hbar}{\tau(E)})/\hbar}\, e^{iS(t)/\hbar}\\
&\quad\times\varphi_0(A(t), B(t), \hbar, a(t), \eta(t), x)\,dt, && (12)
\end{aligned}$$

where θ denotes the conserved quantity

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

and the branch of the square root in (4) is determined by continuity in t. Then, $\Psi(\hbar, x)$ and $E(\hbar) = E + \pi\hbar/\tau(E)$ are a quasimode/quasi-energy pair for $H(\hbar)$, i.e.,

$$\|\Psi(\hbar, \cdot)\| = 1 + O(\hbar^{1/2})$$

and there is a constant C such that

$$\left\| \left[H(\hbar) - \left(E + \frac{\pi\hbar}{\tau(E)} \right) \right] \Psi(\hbar, \cdot) \right\| \leq C\hbar^{3/2} \, \|\Psi(\hbar, \cdot)\| \, . \tag{13}$$

In [10], Paul and Uribe use an integral containing a certain coherent state to produce similar results (in fact, the quasimode and quasi-energy are expanded to all orders in $\hbar$) for one-dimensional Schrödinger operators having polynomial symbols. Karasëv [8] obtains results similar to ours and to the leading terms in [10] using coherent states integrated over arbitrary Lagrangian manifolds. De Bièvre *et al.* [2], [3] use integration of a coherent state along a classical trajectory to obtain approximate eigenfunctions for n-dimensional harmonic oscillators. Our contribution lies in the ideas and methods used in the construction of the quasimode $\Psi(\hbar, x)$. The wave packets used in our construction are semiclassical approximations to the quantum evolution.

The construction detailed in Theorem 1 is easily implemented numerically. Figure 1 compares the absolute square of an exact eigenfunction and our quasimode Ψ for the explicitly solvable Morse potential $V(x) = (1-e^{-x})^2$ [1]. To construct Ψ we took $a_0 = 0$, $\eta_0 = 1$, $A_0 = B_0 = 1$, $n = 10$, and approximated all other necessary quantities using standard numerical schemes. The value of $\hbar$ is 0.0413224 and the quasi-energy $E + \pi\hbar/\tau$ is 0.520682. The tenth eigenvalue above the ground state for the Morse potential with this value of $\hbar$ is 0.519478.

Before proceeding with the proof of the theorem, we present the motivation and intuition that led to our ideas.

1.3 A remark on a "natural" quasimode construction

Integration of an approximate solution of the time–dependent Schrödinger equation over the corresponding classical trajectory is a clear, natural way to attempt to construct a quasimode. However, this naive construction based on the wave packets of [5], [6] fails to work, except in very special cases, such as

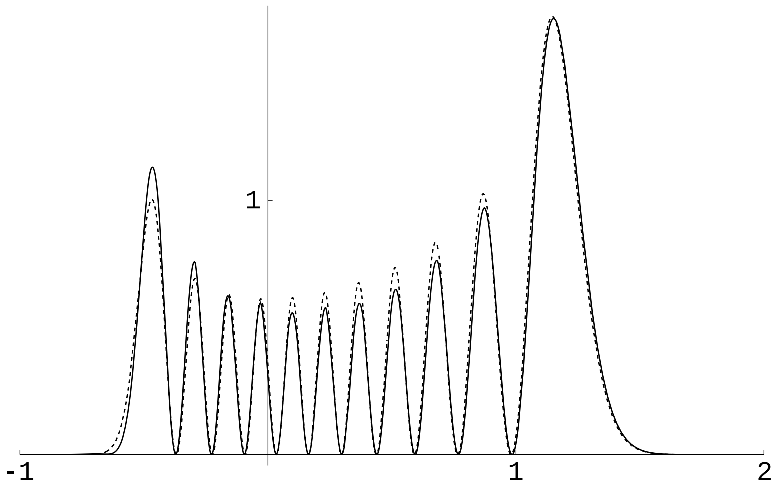

Figure 1: The absolute square of a quasimode (solid line) and the corresponding exact eigenfunction (dashed line) for the Morse potential.

the harmonic oscillator. Understanding this failure provides the motivation for the construction we use.

The wave packets of [5], [6] are the same as those in the theorem, except that $A(t)$ and $B(t)$ satisfy

$$\dot{A}(t) \;=\; iB(t) \tag{14}$$
$$\dot{B}(t) \;=\; iV''(a(t))A(t) \tag{15}$$

instead of (7) and (8). We adopt the shorthand notation

$$\varphi(\hbar,x,t)=\varphi_0(A(t),B(t),\hbar,a(t),\eta(t),x), \tag{16}$$

with $A(t)$ and $B(t)$ satisfying (14) and (15).

The function $e^{iS(t)/\hbar}\varphi(\hbar,x,t)$ is an asymptotic solution of the time-dependent Schrödinger equation in the sense that

$$\left\|e^{-itH(\hbar)/\hbar}\varphi(\hbar,\cdot,0)-e^{iS(t)/\hbar}\varphi(\hbar,\cdot,t)\right\|=O(\hbar^{1/2})$$

and

$$\left\|\left[i\hbar\frac{\partial}{\partial t}-H(\hbar)\right]e^{iS(t)/\hbar}\varphi(\hbar,\cdot,t)\right\|=O(\hbar^{3/2})$$

for $0\le t\le\tau$. The first of these properties is contained in the conclusion of Theorem 1.1 of [6], the second is imbedded in its proof. The branches of the square roots appearing in φ are determined by continuity in t.

The naive approach attempts to construct a quasimode $\Psi \in L^2(\mathbb{R}, dx)$ by

$$\Psi(\hbar, x) = \hbar^{-1/4} \int_0^{\tau(E)} e^{it(E+\frac{\pi\hbar}{\tau(E)})/\hbar} e^{iS(t)/\hbar} \varphi(\hbar, x, t) dt, \tag{17}$$

where the factor of $\hbar^{-1/4}$ is inserted for purposes of normalization. This satisfies

$$\begin{aligned}
&\left(H(\hbar) - E - \frac{\pi\hbar}{\tau(E)}\right) \Psi(\hbar, x) \\
&= \hbar^{-1/4} \int_0^{\tau(E)} \left(H(\hbar) - E - \frac{\pi\hbar}{\tau(E)}\right) \left(e^{it(E+\frac{\pi\hbar}{\tau(E)})/\hbar} e^{iS(t)/\hbar} \varphi(\hbar, x, t)\right) dt \\
&= i\hbar^{3/4} \int_0^{\tau(E)} \frac{\partial}{\partial t} \left(e^{it(E+\frac{\pi\hbar}{\tau(E)})/\hbar} e^{iS(t)/\hbar} \varphi(\hbar, x, t)\right) dt + O(\hbar^{5/4}) \\
&= i\hbar^{3/4} \left(e^{i(\tau E+\pi\hbar+S(\tau))/\hbar} \varphi(\hbar, x, \tau) - \varphi(\hbar, x, 0)\right) + O(\hbar^{5/4}),
\end{aligned} \tag{18}$$

where we have written $F(\hbar, x) = G(\hbar, x) + O(\hbar^p)$ when $\|F(\hbar, \cdot) - G(\hbar, \cdot)\| = O(\hbar^p)$.

If we could arrange for $\varphi(\hbar, x, \tau) = e^{i\rho(\hbar,\tau)/\hbar} \varphi(\hbar, x, 0)$ for some real $\rho(\hbar, \tau)$, then the imposition of the "quantization condition"

$$\tau E + S(\tau) + \pi\hbar + \rho(\hbar, \tau) = 2n\pi\hbar, \; n \in \mathbb{Z}$$

or, its equivalent

$$\oint_{\gamma(E)} p\, dq + \pi\hbar + \rho(\hbar, \tau) = 2n\pi\hbar, \; n \in \mathbb{Z}$$

would lead to Ψ being a quasimode for $H(\hbar)$ because the first term in the last line of (18) would vanish. However, we can use elementary ODE theory (see the proof of the theorem) to show that $B(t+\tau)A^{-1}(t+\tau) \neq B(t)A^{-1}(t)$ for *any* t except in the non–generic special case when $\frac{\partial \tau}{\partial E}(E) = 0$. Thus, the lack of periodicity of the solutions to (14) and (15) causes the naive construction to fail.

Undaunted, we adopt an apparently less natural construction. We seek quasimodes for an operator $f(H)$ rather than H itself. This is not as outlandish as one might think, because spectral mapping arguments relate the spectra of H and $f(H)$, and the classical trajectories are the same for the classical Hamiltonians H and $f(H)$. Furthermore, there is a well-known canonical transformation on phase space (the action-angle variables) that produces dynamics with the period independent of E near a regular trajectory. Although this function of H may be a complicated object with which to work, we can approximate it by its Taylor series to obtain a simpler Hamiltonian.

These ideas lead us to consider a Hamiltonian of the form

$$f_E(H) = H + \frac{1}{2}\frac{\tau'(E)}{\tau(E)}(H-E)^2$$

which is (up to an additive, E-dependent, constant and a scaling by $\tau(E)$) the second order Taylor expansion about $H = E$ of the action variable in the well known action-angle formalism of classical mechanics. Applying the techniques of [5] and [6] to this Hamiltonian, we obtain equations (7 - 8) instead of (14 - 15). The solutions to (7 - 8) have the periodicity to make the naïve construction work for $f_E(H)$, *i.e.*, $\Psi(\hbar, x)$ given by (12) satisfies

$$\left\| \left[f_E(H(\hbar)) - E - \frac{\pi\hbar}{\tau(E)} \right] \Psi(\hbar, \cdot) \right\| = O(\hbar^{3/2}),$$

as long as the Bohr-Sommerfeld quantization condition is satisfied. We then use spectral mapping arguments to prove the theorem.

2 The Proof of the Theorem

The proof of the theorem follows the following outline: First, we develop the necessary classical mechanics. Next, we prove some results on the semiclassical evolution of our Gaussian wave packets. Then, we construct a quasimode for the Hamiltonian $f_E(H(\hbar))$. Finally, we argue that the construction actually yields quasimodes for $H(\hbar)$.

2.1 Some classical quantities

In this section, we establish and collect some facts about classical quantities that arise from two Hamiltonian systems. The first is the standard Newtonian system with Hamiltonian

$$H(q,p) = \frac{1}{2}p^2 + V(q). \tag{19}$$

It is well known (see, *e.g.*, [4]) that for any initial conditions $(q_0, p_0) \in \mathbb{R}^2$ the system

$$\begin{aligned} \dot{q} &= \frac{\partial H}{\partial p}(q,p) = p & (20) \\ \dot{p} &= -\frac{\partial H}{\partial q}(q,p) = -V'(q) & (21) \end{aligned}$$

has a unique solution $(q(q_0, p_0, t),\ p(q_0, p_0, t))$ that satisfies

$$(q(q_0, p_0, 0),\ p(q_0, p_0, 0)) = (q_0, p_0).$$

We often drop the explicit dependence on the initial conditions for convenience, even though much of this section is devoted to studying quantities generated by differentiation with respect to initial conditions. We restrict attention to initial conditions (q_0, p_0) that are contained in a regular trajectory $\gamma(H(q_0, p_0))$. Our study of this system mainly concerns the relations between the derivatives of the solution of (20-21) with respect to initial conditions evaluated at the initial time and at the period of the motion.

We are also interested in the system with Hamiltonian $f_E(H(q,p))$ where

$$f_E(H) = H + \frac{1}{2}\frac{\tau'(E)}{\tau(E)}(H-E)^2. \tag{22}$$

Here, E is considered a parameter and $\tau(E)$ denotes the period of the solution of (20-21) with initial conditions (q_0, p_0) satisfying $H(q_0, p_0) = E$. We introduce this Hamiltonian because derivatives with respect to initial conditions of certain solutions of the resulting Hamiltonian system are periodic with the same period as the orbit. This forces periodicity on certain quasiclassical quantities (namely, $A(t)$ and $B(t)$) that arise in our construction. For the purpose of distinguishing the classical motions generated by the two Hamiltonians, we denote by $((a(a_0, \eta_0, t), \eta(a_0, \eta_0, t))$ the solution of the Hamiltonian system arising from (22):

$$\begin{aligned} \dot{a} &= \frac{\partial}{\partial \eta} f_E(H(a,\eta)) = f_E'(H(a,\eta))\eta & (23) \\ \dot{\eta} &= -\frac{\partial}{\partial a} f_E(H(a,\eta)) = -f_E'(H(a,\eta))V'(a). & (24) \end{aligned}$$

We note that, if $H(a_0, \eta_0) = E$, then

$$((a(a_0, \eta_0, t), \eta(a_0, \eta_0, t)) = (q(a_0, \eta_0, t), p(a_0, \eta_0, t)),$$

i.e., the two motions are identical for all time. As mentioned before, the distinction between these two systems is in the behavior of the derivatives of the motions with respect to initial conditions. It is this behavior we now begin to document.

The existence and time differentiability of the first order partial derivatives of q, p, a, and η with respect to the initial conditions follows from standard ODE theory (see, *e.g.*, [12]). We first concentrate on the system with Hamiltonian (19). Differentiating (20-21) with respect to $r \in \{q_0, p_0\}$, we see that the first order derivatives of q and p satisfy the system

$$\frac{d}{dt}\begin{bmatrix} \frac{\partial q}{\partial r} \\ \frac{\partial p}{\partial r} \end{bmatrix} = M(t)\begin{bmatrix} \frac{\partial q}{\partial r} \\ \frac{\partial p}{\partial r} \end{bmatrix} \tag{25}$$

where $M(t)$ denotes the matrix

$$M(t) = \begin{bmatrix} 0 & 1 \\ -V''(q(t)) & 0 \end{bmatrix}.$$

A fundamental matrix for (25) is

$$U(t) = \begin{bmatrix} \frac{\partial q}{\partial q_0} & \frac{\partial q}{\partial p_0} \\ \frac{\partial p}{\partial q_0} & \frac{\partial p}{\partial p_0} \end{bmatrix},$$

i.e., $\dot{U}(t) = M(t)U(t)$ and $U(0) = I$. We let $\tau = \tau(E)$ (where $E = H(q_0, p_0)$) denote the period of $(q(t), p(t))$, and differentiate both sides of

$$\begin{bmatrix} q(q_0, p_0, t+\tau) \\ p(q_0, p_0, t+\tau) \end{bmatrix} = \begin{bmatrix} q(q_0, p_0, t) \\ p(q_0, p_0, t) \end{bmatrix}$$

with respect to q_0 and p_0 to obtain:

$$U(t+\tau) = U(t) + \tau'(E)\begin{bmatrix} -V'(q_0)p(t) & -p(t)p_0 \\ V'(q(t))V'(q_0) & V'(q(t))p_0 \end{bmatrix}. \tag{26}$$

We now turn our attention to the system generated by the Hamiltonian (22). Differentiating (23-24) with respect to $r \in \{a_0, \eta_0\}$ and restricting to $E = H(a_0, \eta_0)$, we obtain

$$\frac{d}{dt}\begin{bmatrix} \frac{\partial a}{\partial r} \\ \frac{\partial \eta}{\partial r} \end{bmatrix} = M(t)\begin{bmatrix} \frac{\partial a}{\partial r} \\ \frac{\partial \eta}{\partial r} \end{bmatrix} + \frac{\tau'(E)}{\tau(E)}\frac{\partial E}{\partial r}\begin{bmatrix} \eta \\ -V'(a) \end{bmatrix}. \tag{27}$$

Using variation of parameters (and the fact that the nonhomogeneous term actually satisfies the homogeneous part of the equation), we see that

$$\begin{bmatrix} \frac{\partial a}{\partial r} \\ \frac{\partial \eta}{\partial r} \end{bmatrix} = U(t) \begin{bmatrix} \frac{\partial a_0}{\partial r} \\ \frac{\partial \eta_0}{\partial r} \end{bmatrix} + t \frac{\tau'(E)}{\tau(E)} \frac{\partial E}{\partial r} \begin{bmatrix} \eta \\ -V'(a) \end{bmatrix}. \tag{28}$$

This establishes a formula for comparing the solutions of (25) and (27):

$$\begin{bmatrix} \frac{\partial a}{\partial r} \\ \frac{\partial \eta}{\partial r} \end{bmatrix} = \begin{bmatrix} \frac{\partial q}{\partial r} \\ \frac{\partial p}{\partial r} \end{bmatrix} + t \frac{\tau'(E)}{\tau(E)} \frac{\partial E}{\partial r} \begin{bmatrix} p \\ -V'(q) \end{bmatrix}.$$

Evaluating (28) at time $t + \tau(E)$ and using (26), we see that

$$\begin{bmatrix} \frac{\partial a}{\partial r}(t+\tau(E)) \\ \frac{\partial \eta}{\partial r}(t+\tau(E)) \end{bmatrix} = \begin{bmatrix} \frac{\partial a}{\partial r}(t) \\ \frac{\partial \eta}{\partial r}(t) \end{bmatrix} \tag{29}$$

if $H(a_0, \eta_0) = E$.

We now list some simple facts that we use in the next section. We first note that equation (28) implies

$$\eta(t) = \frac{\partial a}{\partial a_0}\eta_0 - \frac{\partial a}{\partial \eta_0} V^{'}(a_0), \tag{30}$$

$$V'(a(t)) = \frac{\partial \eta}{\partial \eta_0} V^{'}(a_0) - \frac{\partial \eta}{\partial a_0}\eta_0. \tag{31}$$

Next, we differentiate $H(a_0, \eta_0) = H(a, \eta)$ with respect to a_0 and η_0 to obtain

$$\begin{aligned} \eta_0 &= \frac{\partial \eta}{\partial \eta_0}\eta(t) + \frac{\partial a}{\partial \eta_0} V^{'}(a(t)), \\ V^{'}(a_0) &= \frac{\partial \eta}{\partial a_0}\eta(t) + \frac{\partial a}{\partial a_0} V^{'}(a(t)). \end{aligned} \tag{32}$$

2.2 The semiclassical evolution and a quasimode for $f_E(H(\hbar))$

We now turn our attention to the quantities A, and B that arise from the solution of (7-8) with $E = H(a_0, \eta_0)$. We first note that the quantity

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

is conserved by the motion generated by (5-8), *i.e.*,

$$\theta(t) = \theta \equiv V'(a_0)A_0 + i\eta_0 B_0.$$

It is easy to see that the two vectors

$$\begin{bmatrix} A(t) \\ iB(t) \end{bmatrix} \qquad \text{and} \qquad \begin{bmatrix} \frac{\partial a}{\partial a_0} \\ \frac{\partial \eta}{\partial a_0} \end{bmatrix} A_0 + i \begin{bmatrix} \frac{\partial a}{\partial \eta_0} \\ \frac{\partial \eta}{\partial \eta_0} \end{bmatrix} B_0$$

both satisfy

$$\frac{d}{dt}\vec{x}(t) = M(t)\vec{x}(t) + \frac{\tau'(E)}{\tau(E)}\theta \begin{bmatrix} \eta \\ -V'(a) \end{bmatrix},$$

with $\vec{x}(0) = \begin{bmatrix} A_0 \\ iB_0 \end{bmatrix}$. So, we conclude that

$$A(t) = \frac{\partial a}{\partial a_0}A_0 + i\frac{\partial a}{\partial \eta_0}B_0$$

and

$$B(t) = \frac{\partial \eta}{\partial \eta_0}B_0 - i\frac{\partial \eta}{\partial a_0}A_0.$$

From these relations and (29), we see that $A(t)$ and $B(t)$ are periodic with period $\tau(E)$.

One can easily check that

$$\overline{A(t)}B(t) + A(t)\overline{B(t)} = \overline{A_0}B_0 + A_0\overline{B_0},$$

so, if A_0 and B_0 satisfy (3), then so do $A(t)$ and $B(t)$ for all $t > 0$.

To determine the phase of $(A(\tau))^{1/2}$ we need to show that the trajectory $\{A(t) : 0 \le t \le \tau\} \subset \mathbb{C}$ has winding number about the origin equal to one. To prove this, we first note that since

$$A(t) = A_0\left[\left(\frac{\partial a}{\partial a_0} - \operatorname{Im}(\frac{B_0}{A_0})\frac{\partial a}{\partial \eta_0}\right) + \frac{i}{|A_0|^2}\frac{\partial a}{\partial \eta_0}\right],$$

it suffices to prove the trajectory $(|A_0|^2\,(\frac{\partial a}{\partial a_0} - \operatorname{Im}(\frac{B_0}{A_0})\frac{\partial a}{\partial \eta_0}), \frac{\partial a}{\partial \eta_0})$ in $\mathbb{R}^2$ winds the origin exactly once. We first consider the special case where the classical motion originates at a turning point, say, $(a_0, \eta_0) = (q_-, 0)$. In this case, equation (30) implies

$$\eta(t) = -\frac{\partial a}{\partial \eta_0} V'(q_-)$$

From this, we deduce that $\dfrac{\partial a}{\partial \eta_0}$ vanishes exactly twice, namely at $t = 0$ and $t = \tau/2$. At $t = 0$,

$$|A_0|^2 \left(\frac{\partial a}{\partial a_0} - \mathrm{Im}(\frac{B_0}{A_0}) \frac{\partial a}{\partial \eta_0} \right) \bigg|_{t=0} = |A_0|^2 > 0$$

and, at $t = \tau/2$,

$$|A_0|^2 \left(\frac{\partial a}{\partial a_0} - \mathrm{Im}(\frac{B_0}{A_0}) \frac{\partial a}{\partial \eta_0} \right) \bigg|_{t=\tau/2} = |A_0|^2 \left. \frac{\partial a}{\partial a_0} \right|_{t=\tau/2} < 0,$$

since equation (32), evaluated at $t = \tau/2$, states

$$\left. \frac{\partial a}{\partial a_0} \right|_{t=\tau/2} V'(q_+) = V'(q_-).$$

From (27) and (31) evaluated at $t = \tau/2$ we find

$$\left. \frac{d}{dt} \frac{\partial a}{\partial \eta_0} \right|_{t=\tau/2} = \left. \frac{\partial \eta}{\partial \eta_0} \right|_{t=\tau/2} = \frac{V'(q_+)}{V'(q_-)} < 0,$$

so $\frac{\partial a}{\partial \eta_0}$ changes sign at $t = \tau/2$ and the claim follows. In the general case, for arbitrary (a_0, η_0) we let t^* denote the first positive time at which the trajectory $(a(t), \eta(t))$ reaches $(q_-, 0)$. By existence and uniqueness, we then have

$$\begin{aligned} A(A_0, B_0, a_0, \eta_0, t + t^*) &= \frac{\partial a}{\partial a_0}(q_-, 0, t) A(t^*) + i \frac{\partial a}{\partial \eta_0}(q_-, 0, t) B(t^*), \\ \eta(a_0, \eta_0, t + t^*) &= -\frac{\partial a}{\partial \eta_0}(q_-, 0, t) V'(q_-), \end{aligned}$$

and the result follows by using the argument for the special case. Hence, if we determine the branch of the square root along the trajectory $\{A(t) : 0 \leq t \leq \tau\}$ by continuity and use $\sqrt{\cdot}$ to denote any fixed branch, we have

$$[A_0]^{1/2} = \sqrt{A_0} \quad \text{implies} \quad [A(\tau(E))]^{1/2} = e^{i\pi} \sqrt{A(\tau(E))}.$$

We note that the phase $e^{i\pi}$ that occurs here is directly related to the Maslov index of the orbit.

We are now nearly ready to develop the semiclassical evolution of the state $\varphi_0(A, B, \hbar, a, \eta, x)$ determined by the Hamiltonian $f_E(H)$. We use the following result to control the semiclassical errors (see Lemma 3.3 of [7]).

Proposition 2 *Let $H(\hbar)$ be a family of self-adjoint operators for $\hbar > 0$. Suppose $\psi(\hbar, x, t)$ is continuously differentiable in t and belongs to the domain of $H(\hbar)$ for $\hbar > 0$. Suppose further that $\psi(\hbar, x, t)$ satisfies:*

$$\left\| \left[i\hbar \frac{\partial}{\partial t} - H(\hbar) \right] \psi(\hbar, \cdot, t) \right\| = O(\hbar^{\lambda})$$

for $t \in [0, T]$. Then

$$\left\| e^{-itH(\hbar)/\hbar} \psi(\hbar, \cdot, 0) - \psi(\hbar, \cdot, t) \right\| = O(\hbar^{\lambda - 1})$$

for $t \in [0, T]$.

To estimate norms that arise in our proof, we rely on the following fact that is easily established by explicit calculation or a scaling argument.

Proposition 3 *If $F(\hbar, x)$ is such that*

$$|F(\hbar, x)| \leq C \hbar^k (x - a)^m$$

for some constants C, k, and non-negative integer m, then

$$\|F(\hbar, \cdot) \varphi_n(A, B, \hbar, a, \eta, \cdot)\| = O(\hbar^{k + m/2}). \tag{33}$$

Moreover, the estimate (33) is uniform for a, η, A, and B in compact sets.

Now, with all quantities defined as in Theorem 1, we define

$$\varphi(\hbar, x, t) = \varphi_0(A(t), B(t), \hbar, a(t), \eta(t), x)$$

with the branches of the square roots appearing in the definition of φ_0 determined by continuity in t starting with a given branch at $t = 0$. Explicit calculation and Proposition 3 show that

$$\left\| \left[i\hbar \frac{\partial}{\partial t} - f_E(H(\hbar)) \right] e^{iS(t)/\hbar} \varphi(\hbar, \cdot, t) \right\| = O(\hbar^{3/2}). \tag{34}$$

By Proposition 2, this implies that

$$\left\| e^{-itf_E(H(\hbar))/\hbar}\varphi(\hbar,\cdot,0) - e^{iS(t)/\hbar}\varphi(\hbar,\cdot,t)\right\| = O(\hbar^{1/2}).$$

The argument from Section 1.3 then shows that

$$\Psi(\hbar,x) = \hbar^{-1/4}\int_0^{\tau(E)} e^{it(E+\frac{\pi\hbar}{\tau(E)})/\hbar} e^{iS(t)/\hbar}\varphi(\hbar,x,t)\,dt$$

satisfies

$$\begin{aligned}
&\left[f_E(H(\hbar)) - E - \frac{\pi\hbar}{\tau(E)}\right]\Psi(\hbar,x) \\
&\qquad = i\hbar^{3/4}\left(e^{i(\tau E+\pi\hbar+S(\tau))/\hbar}\varphi(\hbar,x,\tau) - \varphi(\hbar,x,0)\right) + O(\hbar^{5/4}). \qquad (35)
\end{aligned}$$

Using the facts in the beginning of this section we conclude

$$\varphi(\hbar,x,\tau) = e^{-i\pi}\varphi(\hbar,x,0),$$

and therefore,

$$e^{i(\tau E+\pi\hbar+S(\tau))/\hbar}\varphi(\hbar,x,\tau) - \varphi(\hbar,x,0) = 0$$

if

$$\tau E + S(\tau) = 2n\pi\hbar \qquad (36)$$

for some integer n. This is precisely the Bohr–Sommerfeld condition (11). To see this, note that by using time to parametrize the integral

$$I(E) = \oint_{\gamma(E)} p\,dq,$$

and using $\dfrac{\partial q}{\partial t} = p$, we have

$$\begin{aligned}
I(E) &= \int_0^{\tau(E)} p(t)^2\,dt \\
&= \int_0^{\tau(E)} \left(p(t)^2/2 + V(q(t))\right)\,dt + \int_0^{\tau(E)} \left(p(t)^2/2 - V(q(t))\right)\,dt \\
&= E\,\tau(E) + S(\tau(E)).
\end{aligned}$$

Thus, if we restrict the values of $\hbar$ to the sequence

$$\hbar \in \left\{ \frac{I(E)}{2\pi n} \right\}_{n \in \mathbb{Z}^+}$$

we have

$$\left[f_E(H(\hbar)) - E - \frac{\pi\hbar}{\tau(E)} \right] \Psi(\hbar, x) = O(\hbar^{5/4}). \tag{37}$$

In the next section, we prove that the norm of Ψ is of order 1. Thus, (37) shows that Ψ and $E + \pi\hbar/\tau(E)$ are a quasimode/quasi-energy pair for the Hamiltonian $f_E(H(\hbar))$. We also show in the next section that the power of $\hbar$ on the right side of equation (37) can be improved to 3/2.

2.3 The normalization of Ψ and an improved error estimate

In this section, we prove some estimates which allow us to show that our quasimode Ψ is properly normalized and that the error in equation (37) is actually $O(h^{3/2})$.

We need two preliminary results. We first obtain a formula for the inner product of two Gaussians of the form (4), that is proved by explicit integration.

Proposition 4 *Suppose the pair A_1 and B_1 satisfy (3) and the pair A_2 and B_2 satisfy (3). Suppose a_1, η_1, a_2, and η_2 are real, and let $\hbar$ be positive. Then*

$$\begin{aligned} &\langle \varphi_0(A_1, B_1, \hbar, a_1, \eta_1, \cdot), \varphi_0(A_2, B_2, \hbar, a_2, \eta_2, \cdot) \rangle = \\ &\qquad \sqrt{\frac{2}{B_2\overline{A_1} + A_2\overline{B_1}}} \exp\left\{ -\frac{A_2\overline{A_1}(\eta_2 - \eta_1)^2 + B_2\overline{B_1}(a_2 - a_1)^2}{2\hbar(B_2\overline{A_1} + A_2\overline{B_1})} \right. \\ &\qquad\qquad \left. - i\frac{(a_2 - a_1)(B_2\overline{A_1}\eta_1 + A_2\overline{B_1}\eta_2)}{\hbar(B_2\overline{A_1} + A_2\overline{B_1})} \right\}. \end{aligned}$$

Next, we prove an estimate that concerns integrals of a type we encounter.

Proposition 5 *Suppose $f(t,s)$ is a complex C^2 function and $g(t,s)$ is a complex C^3 function, for $t \in [0,T]$ and $s \in [-T/2, T/2]$. Suppose there exists $\delta > 0$, such that* $\mathrm{Re}(g(t,s)) \geq \delta s^2$, *for $t \in [0,T]$ and $s \in [-T/2, T/2]$;*

$g(t,0)=0$; $\dfrac{\partial g}{\partial s}(t,0)=0$; *and* $\dfrac{\partial^2 g}{\partial s^2}(t,0)=\alpha(t)$ *is real and positive. Then for any non-negative integer* n, *we have*

$$\int_0^T dt \int_{-T/2}^{T/2} ds\, f(t,s)s^{2n}e^{-g(t,s)/\hbar} = \\ 1\cdot 3\cdots|2n-1|\,\sqrt{2\pi}\;\hbar^{n+1/2}\int_0^T f(t,0)\alpha(t)^{-n-1/2}dt + O(\hbar^{n+1}).$$

Proof: On the domain of interest, $|f(t,s)|$ is uniformly bounded by some number C_1. Because $\operatorname{Re} g(t,s)\geq \delta s^2$, we have $|e^{-g(t,s)/\hbar}|\leq e^{-\delta s^2/\hbar}$. Thus, $|s|>\hbar^\gamma$ implies

$$\left|f(t,s)s^{2n}e^{-g(t,s)/\hbar}\right| \leq C_1(T/2)^{2n}e^{-\delta/\hbar^{1-2\gamma}}.$$

Therefore, for any $\gamma<1/2$,

$$\int_0^T dt\int_{\hbar^\gamma<|s|\leq T/2} ds\, f(t,s)s^{2n}e^{-g(t,s)/\hbar}=O(\hbar^p),$$

for any p.

So, the integral in question equals

$$\int_0^T dt\int_{-\hbar^\gamma}^{\hbar^\gamma} ds\, f(t,s)s^{2n}e^{-g(t,s)/\hbar}+O(\hbar^p).$$

Since $\left|e^{-g(t,s)/\hbar}\right|\leq 1$, standard error estimates for first order Taylor series now show that the integral equals

$$\int_0^T dt\int_{-\hbar^\gamma}^{\hbar^\gamma} ds(f(t,0)+\frac{\partial f}{\partial s}(t,0)s)s^{2n}e^{-g(t,s)/\hbar} + \\ \int_0^T dt\int_{-\hbar^\gamma}^{\hbar^\gamma} ds\frac{1}{2}\frac{\partial^2 f}{\partial s^2}(t,\xi(t,s))s^{2n+2}e^{-g(t,s)/\hbar}, \qquad (38)$$

for some $\xi(t,s)$ with values between 0 and s.

Since $\left|\dfrac{1}{2}\dfrac{\partial^2 f}{\partial s^2}(t,\xi(t,s))e^{-g(t,s)/\hbar}\right|$ is bounded by some C_2, the second term in (38) is bounded by $C_2T\hbar^{(2n+3)\gamma}/(2n+3)$. By choosing γ sufficiently close to $1/2$, this can be made $O(\hbar^{n+1})$.

Next, by standard Taylor series error estimates and our hypotheses on g, we have $g(t,s) = \alpha(t)s^2/2 + O(s^3)$, uniformly for $t \in [0,T]$. Thus, $|s| \le \hbar^\gamma$ implies

$$\begin{aligned}\left| e^{-g(t,s)/\hbar} - e^{-\alpha(t)s^2/(2\hbar)} \right| &\le \left| e^{\left(\alpha(t)\frac{s^2}{2} - g(t,s)\right)/\hbar} - 1 \right| e^{-\alpha(t)s^2/(2\hbar)} \\ &\le C_3 \frac{|s|^3}{\hbar} e^{-\alpha(t)s^2/(2\hbar)}.\end{aligned}$$

Since

$$\int_0^T dt \int_{-\hbar^\gamma}^{\hbar^\gamma} ds \left| f(t,0) + \frac{\partial f}{\partial s}(t,0)s \right| \frac{|s|^{2n+3}}{\hbar} e^{-\alpha(t)s^2/(2\hbar)} \le C_4 \hbar^{n+1},$$

the first term in (38) equals

$$\int_0^T dt \int_{-\hbar^\gamma}^{\hbar^\gamma} ds (f(t,0) + \frac{\partial f}{\partial s}(t,0)s) s^{2n} e^{-\alpha(t)s^2/(2\hbar)} + O(\hbar^{n+1}). \qquad (39)$$

We make an exponentially small error by extending the s integration in (39) to the whole real line. We then explicitly compute the resulting s integral to obtain

$$\begin{aligned}&\int_0^T dt \int_{-\hbar^\gamma}^{\hbar^\gamma} ds\, f(t,s) s^{2n} e^{-\alpha(t)s^2/(2\hbar)} = \\ &\qquad 1 \cdot 3 \cdots |2n-1| \sqrt{2\pi}\ \hbar^{n+1/2} \int_0^T f(t,0)\alpha(t)^{-n-1/2} dt + O(\hbar^{n+1}).\end{aligned}$$

This implies the proposition. ■

Now, let $\Psi(\hbar, x)$ be defined as in Theorem 1:

$$\begin{aligned}\Psi(\hbar,x) &= (\pi\hbar)^{-1/4} \sqrt{\frac{|\theta|}{2\tau(E)}} \int_0^{\tau(E)} e^{it(E+\frac{\pi\hbar}{\tau(E)})/\hbar} e^{iS(t)/\hbar} \\ &\quad \times \varphi_0(A(t), B(t), \hbar, a(t), \eta(t), x)\, dt.\end{aligned}$$

Proposition 6 *The norm of the quasimode $\Psi(\hbar, \cdot)$ satisfies*

$$\|\Psi(\hbar, \cdot)\| = 1 + O(\hbar^{1/2}).$$

Proof: The square of the norm of the quasimode is

$$\langle \Psi(\hbar,\,\cdot), \Psi(\hbar,\,\cdot)\rangle = (\pi\hbar)^{-1/2}\frac{|\theta|}{2\tau}\times$$

$$\Big\langle \int_0^\tau e^{-it_2(E+\frac{\pi\hbar}{\tau})/\hbar} e^{-iS(t_2)/\hbar}\varphi_0(A(t_2),B(t_2),\hbar,a(t_2),\eta(t_2),x)\,dt_2,$$

$$\int_0^\tau e^{it_1(E+\frac{\pi\hbar}{\tau})/\hbar} e^{iS(t_1)/\hbar}\varphi_0(A(t_1),B(t_1),\hbar,a(t_1),\eta(t_1),x)\,dt_1\Big\rangle$$

$$= (\pi\hbar)^{-1/2}\frac{|\theta|}{2\tau}\int_0^\tau\int_0^\tau \exp\left\{i\left[S(t_1)-S(t_2)+(t_1-t_2)\left(E_0+\frac{\pi\hbar}{\tau}\right)\right]/\hbar\right\}\times$$

$$\langle\varphi_0(A(t_2),B(t_2),\hbar,a(t_2),\eta(t_2),\cdot),\varphi_0(A(t_1),B(t_1),\hbar,a(t_1),\eta(t_1),\cdot)\rangle\;\;dt_1\,dt_2$$

$$= (\pi\hbar)^{-1/2}\frac{|\theta|}{2\tau}\int_0^\tau dt\int_{-\tau/2}^{\tau/2} ds\;\exp i\left[S(t)-S(t+s)-s\left(E_0+\frac{\pi\hbar}{\tau}\right)\right]/\hbar\times$$

$$\sqrt{\frac{2}{B(t)\overline{A(t+s)}+\overline{B(t+s)}A(t)}}\times$$

$$\exp\left\{-\frac{A(t)\overline{A(t+s)}(\eta(t+s)-\eta(t))^2+B(t)\overline{B(t+s)}(a(t+s)-a(t))^2}{2\hbar(B(t)\overline{A(t+s)}+\overline{B(t+s)}A(t))}\right\}\times$$

$$\exp\left\{-\,i\;\frac{(a(t)-a(t+s))\left(B(t)\overline{A(t+s)}\eta(t+s)+\overline{B(t+s)}A(t)\eta(t)\right)}{\hbar\,(B(t)\overline{A(t+s)}+\overline{B(t+s)}A(t))}\right\}.$$

In the last step we have changed the limits of integration by exploiting periodicity in t_2 and changed variables by $t=t_1$ and $s=t_2-t_1$. We have also used Proposition 4 to evaluate the inner product in the integrand.

We rewrite the integrand in the form $f(t,s)\,e^{-g(t,s)/\hbar}$, where

$$f(t,\,s)=e^{-i\pi s/\tau}\,\sqrt{\frac{2}{B(t)\overline{A(t+s)}+\overline{B(t+s)}A(t)}}.$$

We note that $\mathrm{Re}\,g(t,s)\geq 0$ and $g(t,0)=0$. Also, formula (3) implies $f(t,0)=1$.

Making use of equations (5)–(9), we compute the second order Taylor series expansion of $g(t,s)$ in the variable s. This is a lengthy calculation, but the result is

$$\begin{aligned} g(t,s) &= i\eta(t)V'(a(t))\left(1-B(t)\overline{A(t)}\right)\frac{s^2}{2} \\ &\quad -\left(|A(t)|^2V'(a(t))^2+|B(t)|^2\eta(t)^2\right)\frac{s^2}{4}+O(s^3). \end{aligned}$$

By using formula (3), we can rewrite this as

$$g(t,s) = -\left|A(t)V'(a(t))+iB(t)\eta(t)\right|^2\frac{s^2}{4}+O(s^3)-\frac{|\theta|^2s^2}{4}+O(s^3).$$

It now follows that the hypotheses of Proposition 5 are satisfied. Thus, Proposition 5 and an explicit integration show

$$||\Psi(\hbar,\cdot)||^2 = 1+O(\hbar^{1/2}).$$

The proposition follows by taking square roots. ■

We close this section with an outline of the proof that the error in the estimate (37) is actually of order $\hbar^{3/2}$. The idea is to use a variant of Proposition 4 and Proposition 5 to estimate the right side of (34) rather than bringing the norm inside the integral and using Proposition 3. Explicit calculation shows that the quantity inside the norm in equation (34) is actually

$$\begin{aligned} &\left[i\hbar\frac{\partial}{\partial t}-f_E(H(\hbar))\right]e^{iS(t)/\hbar}\varphi(\hbar,x,t) = \\ &\quad \hbar^{3/2}e^{iS(t)/\hbar}\left(f_1(t)\varphi_1(A(t),B(t),\hbar,a(t),\eta(t),x)\right. \\ &\quad\quad \left.+f_3(t)\varphi_3(A(t),B(t),\hbar,a(t),\eta(t),x)\right)+O(\hbar^2) \end{aligned}$$

where

$$\begin{aligned} \varphi_n(A,B,\hbar,a,\eta,x) &= 2^{-n/2}(\pi\hbar)^{-n/4}A^{-(n+1)/2}\bar{A}^{n/2}H_n(\hbar^{-1/2}\left|A\right|^{-1}(x-a))\times \\ &\quad \exp\left\{-\frac{1}{2\hbar}BA^{-1}(x-a)^2+\frac{i}{\hbar}\eta(x-a)\right\} \end{aligned}$$

with H_n denoting the n^{th} Hermite polynomial and f_1 and f_3 given by rather complicated expressions in $A(t)$, $B(t)$, $a(t)$, $\eta(t)$, $V(a(t))$, and $V^{(n)}(a(t))$ for $n = 1, 2, 3$ which we do not display here. This implies that the $O(\hbar^{5/4})$ term in equation (35) is

$$\hbar^{5/4}\int_0^T e^{it(E+\frac{\pi\hbar}{T})/\hbar}e^{iS(t)/\hbar}(f_1\varphi_1+f_3\varphi_3)(t)dt+O(\hbar^{7/4}).$$

We then estimate the L^2 norm of the integral above using the same trick as in the proof of Proposition 6, *i.e.*,

$$\left\| \int_0^{\tau} e^{it(E+\frac{\pi\hbar}{\tau})/\hbar} e^{iS(t)/\hbar} (f_1\varphi_1 + f_3\varphi_3)(t)dt \right\|^2 =$$
$$\left\langle \int_0^{\tau} e^{it_1(E+\frac{\pi\hbar}{\tau})/\hbar} e^{iS(t_1)/\hbar} (f_1\varphi_1 + f_3\varphi_3)(t_2)dt_2, \right.$$
$$\left. \int_0^{\tau} e^{it_2(E+\frac{\pi\hbar}{\tau})/\hbar} e^{iS(t_2)/\hbar} (f_1\varphi_1 + f_3\varphi_3)(t_1)dt_1 \right\rangle. \quad (40)$$

We break this into four integrals in x, $s = t_2 - t_1$, and $t = t_1$ and bring the inner products "inside the integrals". We then use the following extension of Proposition 4 to evaluate the inner products:

Proposition 7 *Suppose the pair A_1 and B_1 satisfy (3) and the pair A_2 and B_2 satisfy (3). Suppose a_1, η_1, a_2, and η_2 are real, and let $\hbar$ be positive. Then*

$$\langle \varphi_l(A_1, B_1, \hbar, a_1, \eta_1, \cdot), \varphi_k(A_2, B_2, \hbar, a_2, \eta_2, \cdot)\rangle =$$
$$\frac{1}{\sqrt{l!k!}} 2^{-\frac{l+k}{2}} \langle \varphi_0(A_1, B_1, \hbar, a_1, \eta_1, \cdot), \varphi_0(A_2, B_2, \hbar, a_2, \eta_2, \cdot)\rangle \times$$
$$(\overline{B_1}A_2 + \overline{A_1}B_2)^{-\frac{l+k}{2}} \sum_{j=0}^{\min(l,k)} \left[\binom{l}{j}\binom{k}{j} j!4^j (\overline{A_2B_1} - \overline{A_1B_2})^{\frac{k-j}{2}} \times \right.$$
$$(A_1B_2 - A_2B_1)^{\frac{l-j}{2}} H_{k-j}(\hbar^{-1/2} \frac{\overline{B_1}(a_1 - a_2) - i\overline{A_1}(\eta_1 - \eta_2)}{\sqrt{\overline{A_2B_1} - \overline{A_1B_2}}\sqrt{\overline{B_1}A_2 + \overline{A_1}B_2}}) \times$$
$$\left. H_{l-j}(-\hbar^{-1/2} \frac{B_2(a_1 - a_2) + iA_2(\eta_1 - \eta_2)}{\sqrt{A_1B_2 - A_2B_1}\sqrt{\overline{B_1}A_2 + \overline{A_1}B_2}}) \right].$$

Proof: Induction and the properties of the Hermite polynomials establish the integral formula

$$\int_{-\infty}^{\infty} e^{-\rho x^2} H_m(ax+b) H_n(cx+d)\, dx = \sqrt{\pi}\rho^{-\frac{1}{2}(m+n+1)} \times$$
$$\sum_{k=0}^{\min(m,n)} \left[\binom{m}{k}\binom{n}{k} k!(\rho - a^2)^{\frac{m-k}{2}} (\rho - c^2)^{\frac{n-k}{2}} (2ac)^k \times \right.$$
$$\left. H_{m-k}(b\sqrt{\frac{\rho}{\rho - a^2}}) H_{n-k}(d\sqrt{\frac{\rho}{\rho - c^2}}) \right]$$

for $\mathrm{Re}(\rho) > 0$ from which the proposition follows easily by completion of the square in the exponent and a change of variable of integration. ■

This implies that the right side of (40) is a sum of terms of the form

$$\hbar^{-(m+n)/2} \int_0^\tau dt \int_{-\tau/2}^{\tau/2} ds\, f(t,s)\, z_1(t,s)^m\, z_2(t,s)^n e^{-g(t,s)/\hbar} \tag{41}$$

where

$$\begin{aligned} z_1(t,s) &= \overline{B(t)}(a(t) - a(s+t)) - i\overline{A(t)}(\eta(t) - \eta(s+t)), \\ z_2(t,s) &= B(s+t)(a(t) - a(s+t)) + iA(s+t)(\eta(t) - \eta(s+t)), \end{aligned}$$

$m+n$ is an even integer, $f(t,s)$ is a complex C^2 function, and $g(t,s)$ is as in Proposition 6. For any $\gamma < 1/2$, (41) is equal to

$$\hbar^{-(m+n)/2} \int_0^\tau dt \int_{-\hbar^\gamma}^{\hbar^\gamma} ds\, f(t,s)\, z_1(t,s)^m\, z_2(t,s)^n e^{-g(t,s)/\hbar} + O(\hbar^p)$$

for any p. We make an error of order

$$O(\hbar^{-(m+n)/2} \times \hbar^{\gamma(m+n+2)}) = O(\hbar^{2\gamma-(1-2\gamma)(m+n)/2})$$

by replacing $z_1(t,s)$ and $z_2(t,s)$ by their Taylor series in s:

$$\begin{aligned} z_1(t,s) &= -i\overline{\theta}s + O(s^2), \\ z_2(t,s) &= i\theta s + O(s^2), \end{aligned}$$

and an exponentially small error in extending the s integration back to the interval $[-\tau/2, \tau/2]$ to obtain:

$$\begin{aligned} &\hbar^{-(m+n)/2} \int_0^\tau dt \int_{-\tau/2}^{\tau/2} ds\, f(t,s)\, z_1(t,s)^m\, z_2(t,s)^n e^{-g(t,s)/\hbar} = \\ &\qquad \hbar^{-(m+n)/2} \int_0^\tau dt \int_{-\tau/2}^{\tau/2} ds\, f(t,s)\, s^{m+n} e^{-g(t,s)/\hbar} + O(\hbar^{2\gamma-(1-2\gamma)(m+n)/2}) \end{aligned}$$

Proposition 5 now applies with the result that

$$\left\| \int_0^\tau e^{it(E+\frac{\pi\hbar}{\tau})/\hbar} e^{iS(t)/\hbar} (f_1\varphi_1 + f_3\varphi_3) dt \right\| = O(h^{1/4})$$

for sufficiently large γ, and hence the right side of equation (35) is actually

$$i\hbar^{3/4} \left(e^{i(\tau E + \pi\hbar + S(\tau))/\hbar} \varphi(\hbar, x, \tau) - \varphi(\hbar, x, 0) \right) + O(\hbar^{3/2}),$$

thus providing us with the estimate necessary to prove (13).

2.4 A quasimode for H

In this section we complete the proof of the theorem. We must establish the connection between quasimodes for the Hamiltonian $f_E(H(\hbar))$ and quasimodes for the Hamiltonian $H(\hbar)$. We cannot establish this by use of spectral mapping arguments alone, because the map $x \mapsto f_E(x)$ is not invertible. This complication is easily overcome, however, with use of the following observations:

1. Our quasimode Ψ for $f_E(H)$ is also a quasimode for the Hamiltonian

$$g_E(H) = H + \frac{1}{2}\frac{\tau'(E)}{\tau(E)}(H-E)^2 + \beta(H-E)^3$$

for *arbitrary* $\beta \in \mathbb{R}$. This follows because the crucial estimate (34) (and hence, every result in the preceding two sections) holds with $f_E(H(\hbar))$ replaced with $g_E(H(\hbar))$ for arbitrary $\beta \in \mathbb{R}$.

2. If $\beta > \alpha^2/3$, the polynomial function $p(x) = x + \alpha x^2 + \beta x^3$ on $\mathbb{R}$ has an inverse. This follows by showing that, for such values of β, $p'(x) > 0$ for all $x \in \mathbb{R}$.

Armed with these two simple observations, we now settle the question of relating quasimodes of $f_E(H(\hbar))$ (or $g_E(H(\hbar))$) to quasimodes of $H(\hbar)$.

Proposition 8 *Suppose $H(\hbar)$ is self-adjoint on a Hilbert space $\mathcal{H}$, and $E \in \mathbb{R}$. Suppose $g(z) = z + \alpha(z-E)^2 + \beta(z-E)^3$, where β is chosen large enough so that $g(z+E) - E$ is invertible. Suppose there exists a vector $\psi(\hbar) \in \mathcal{H}$ with $\|\psi(\hbar)\| = 1$, such that $\|[g(H(\hbar)) - E]\,\psi(\hbar)\,\| \le C\,\hbar^\lambda$ for some $\lambda > 0$. Then there exists C', such that*

$$\|[H(\hbar) - E]\psi(\hbar)\| \le C'\hbar^\lambda.$$

Proof: We define $g_1 : \mathbb{R} \to \mathbb{R}$ by

$$g_1(z) = g(z+E) - E = z + \alpha z^2 + \beta z^3,$$

and let h be its inverse function. Clearly, h is differentiable; $h(0) = 0$; and $|h(z)|$ grows at most linearly for large $|z|$. Thus, there exists C'', such that $|h(z)| \le C''\,|z|$ for all $z \in \mathbb{R}$.

By the spectral theorem, there exists a unitary operator $U_\hbar$ from $\mathcal{H}$ to the direct sum $\bigoplus_j L^2(\mathbb{R}, d\mu_{\hbar,j}(x))$, such that $U_\hbar H(\hbar) U_\hbar^{-1}$ is multiplication by x.

Letting $\phi_{\hbar,j}(\cdot)$ denote the j^{th} component of $U_\hbar \psi(\hbar)$, we have

$$\begin{aligned}
\|[H(\hbar)-E]\psi(\hbar)\|^2 &= \sum_j \int_{\mathbb{R}} |x-E|^2\, |\phi_{\hbar,j}(x)|^2\, d\mu_{\hbar,j}(x) \\
&= \sum_j \int_{\mathbb{R}} |h(g_1(x-E))|^2\, |\phi_{\hbar,j}(x)|^2\, d\mu_{\hbar,j}(x) \\
&\le \sum_j \int_{\mathbb{R}} C''^2\, |g_1(x-E)|^2\, |\phi_{\hbar,j}(x)|^2\, d\mu_{\hbar,j}(x) \\
&= C''^2\, \|\, g_1(H(\hbar)-E)\, \psi(\hbar)\,\|^2 \\
&= C''^2\, \|\, [g(H(\hbar))-E]\, \psi(\hbar)\,\|^2 \\
&\le C''^2\, C^2\, \hbar^{2\lambda}.
\end{aligned}$$

This implies the proposition with $C' = C''\, C$. ■

References

[1] J. P. Dahl and M. Springborg, "The Morse oscillator in position space, momentum space, and phase space", *J. Chem. Phys.*, **88** (7), p. 4535-4547, 1988.

[2] S. De Bièvre, "Oscillator eigenstates concentrated on classical trajectories," *J. Phys. A*, **25**, p. 3390–3418, 1992.

[3] S. De Bièvre, J. C. Hourd, and M. Irac-Astaud, "Wave packets localized on closed classical trajectories," in *Differential Equations with Applications to Mathematical Physics*, Mathematics in Science and Engineering, Volume 192, edited by W. F. Ames, E. M. Harrell II, and J. V. Herod, Academic Press, San Diego, 1993.

[4] G. Gallavoti, *The Elements of Mechanics*, Springer-Verlag, New York, 1983.

[5] G. Hagedorn, "Semiclassical quantum mechanics I: the $\hbar \to 0$ limit for coherent states," *Commun. Math. Phys.*, **71**, p. 77-93, 1980.

[6] G. Hagedorn, "Semiclassical quantum mechanics III: the large order asymptotics and more general states," *Ann. Phys*, **135**, p. 58-70, 1981.

[7] G. Hagedorn, *Molecular Propagation through Electron Energy Level Crossings*, Memoirs of the American Mathematical Society, Volume 111, Number 536, American Mathematical Society, Providence, Rhode Island, 1994.

[8] M. V. Karasëv, "Simple quantization formula," in *Symplectic Geometry and Mathematical Physics (Aix-en-Provence 1990),* Progress in Mathematics, Volume 99, Birkhäuser, Boston, 1991.

[9] M. D. Khaut-Duy, "Formule des traces semi-classique pour une énergie critique et construction de quasi-modes à l'aide d'états cohérents", doctoral thesis, Universite Paris IX Dauphine, 1996.

[10] T. Paul and A. Uribe, "A construction of quasi-modes using coherent states," *Ann. Inst. Henri Poincaré*, Vol. 59, n^o 4, p. 357-381, 1993.

[11] T. Paul and A. Uribe, "On the pointwise behavior of semi–classical measures," *Commun. Math. Phys.*, **175**, p. 229–258, 1996.

[12] L. C. Piccini, G. Stampacchia, and G. Vidossich, *Ordinary Differential Equations in* R^n, Applied Mathematical Sciences **39**, Springer-Verlag, New York, 1984.

[13] J. V. Ralston, "On the construction of quasimodes associated with stable periodic orbits," *Commun. Math. Phys.,* **51**, p. 219-242, 1976.