Exponentially Accurate Quasimodes for the Time–Independent Born–Oppenheimer Approximation on a One–Dimensional Molecular System

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Abstract

We consider the eigenvalue problem for a one-dimensional molecular–type quantum Hamiltonian that has the form

$$H(\epsilon) \;=\; -\,\frac{\epsilon^4}{2}\,\frac{\partial^2}{\partial y^2} \;+\; h(y),$$

where $h(y)$ is an analytic family of self-adjoint operators that has an discrete, nondegenerate electronic level $\mathcal{E}(y)$ for y in some open subset of $\mathbb{R}$. Near a local minimum of the electronic level $\mathcal{E}(y)$ that is not at a level crossing, we construct quasimodes that are exponentially accurate in the square of the Born–Oppenheimer parameter ϵ by optimal truncation of the Rayleigh–Schrödinger series. That is, we construct an energy E_ϵ and a wave function Ξ_ϵ, such that the L^2-norm of Ξ_ϵ is $\mathcal{O}(1)$ and the L^2-norm of $(H(\epsilon) - E_\epsilon)\,\Xi_\epsilon$ is bounded by $\Lambda\,\exp\big(-\Gamma/\epsilon^2\big)$ with $\Gamma > 0$.

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1 Introduction

In this paper we construct exponentially accurate quasimodes for the time–independent Schrödinger equation for a simple molecular system. The small parameter that governs the approximation is the usual Born–Oppenheimer parameter ϵ, where ϵ^4 is the electron mass divided by the mean nuclear mass. Under appropriate circumstances, the quasimodes we produce correspond exactly to the low–lying energy levels of the system. In that case, the exact eigenvalues and our quasimode energies differ by at most $\Lambda \exp\left(-\Gamma/\epsilon^2\right)$. A bound of the same form holds for the norm of the difference between the quasimodes and the exact eigenvectors.

Hamiltonians for molecular systems can generally be put in the form

$$H(\epsilon) \;=\; -\,\frac{\epsilon^4}{2}\,\Delta_y \;+\; h(y),$$

where the variable y describes the nuclear configuration vector and the operator $h(y)$ is the electron Hamiltonian. In this paper we examine the special case of operators of this type, where y is a single real variable, and $h(y)$ is a family of (possibly unbounded) self–adjoint operators. There are three motivations for studying this somewhat unphysical model. First, few rigorous exponentially accurate results for the time–independent Born–Oppenheimer approximation have been published, and they do not cover this model. Indeed, the only previous results of this kind, to the best of our knowledge, is our study of the special case where $h(y)$ is a 2×2 real symmetric matrix [9]. Second, we consider the treatment of this model as an intermediate stage toward the study of more realistic molecular systems. We hope to be able to construct exponentially accurate quasimodes for diatomic molecules, using the techniques developed in [9] and in this paper, although several technical difficulties are yet to be overcome. Finally, we believe that the results we present are nevertheless interesting in themselves, because they generalize those of [9] to a much larger class of situations with a relatively small amount of work. Most of the heavy computations have been done in [9]. Although the technical details are somewhat different, we essentially reduce the present problem to the one studied in [9].

To state our results precisely, we need some notation and hypotheses. For small ϵ, we study the eigenvalue problem

$$\left[-\frac{\epsilon^4}{2}\,\frac{d^2}{dy^2} \,+\, h(y)\right]\,\Psi(\epsilon,\,y) \;=\; E(\epsilon)\;\Psi(\epsilon,\,y),$$

where $h(y)$ denotes a family of operators that satisfies the following conditions:

1. $h(y) : \mathcal{H}_e \to \mathcal{H}_e$ is a self–adjoint operator for every $y \in \mathbb{R}$, where the electronic Hilbert space $\mathcal{H}_e$ is separable. We furthermore assume that $\inf \sigma(h(y))$ is uniformly bounded from below.

2. $h(y)$ is an analytic family of type (A) in a neighborhood $S \subset \mathbb{C}$ of the origin. From hypothesis 1, it follows that $h(y)^\star = h(\overline{y})$ for $y \in S$.

3. We assume $h(0)$ has an isolated, non-degenerate eigenvalue $\mathcal{E}(0)$.

By standard results, these hypotheses imply that $h(y)$ has an isolated, non-degenerate eigenvalue $\mathcal{E}(y)$ that depends analytically on y in a neighborhood $S' \subset S$ of the origin. The associated projection $P(y)$ is analytic for $y \in S'$, and it is orthogonal for real y. The y-independent domain D of $h(y)$ is a dense subspace of the electronic Hilbert space $\mathcal{H}_e$. Finally we assume:

4. $\mathcal{E}(y)$ has a non-degenerate local minimum at $y = 0$, *i.e.*, $\mathcal{E}'(0) = 0$ and $\mathcal{E}''(0) > 0$. Without loss we assume that $\mathcal{E}(0) = 0$ and $\mathcal{E}''(0) = 1$.

An eigenfunction $\Psi(\epsilon, y)$ of $H(\epsilon)$ belongs to $L^2(\mathbb{R}, \mathcal{H}_e)$, whose norm we denote by $|||\cdot|||$.

Under these hypotheses, we have the following result:

Theorem 1 *Assume hypotheses 1–4, and let α be a fixed non-negative integer. Then, using optimal truncation of a perturbation expansion in powers of ϵ, we can construct E_ϵ and Ξ_ϵ, such that $|||\,\Xi_\epsilon\,||| \,=\, \mathcal{O}(1)$, $\quad E_\epsilon \,=\, (\alpha + 1/2)\,\epsilon^2 \,+\, \mathcal{O}(\epsilon^4)$, and*

$$|||\,(H(\epsilon) - E_\epsilon)\,\Xi_\epsilon\,||| \;<\; \Lambda\,\exp\,\left(-\,\Gamma/\epsilon^2\right).$$

This quasimode is associated with the α^{th} vibrational energy level in the local well of $\mathcal{E}$ near $y = 0$.

Remarks. **1.** Our hypotheses allow level crossings as well as merging of $\mathcal{E}$ into the continuous spectrum, as long as these phenomena do not occur at the bottom of the local well of $\mathcal{E}$ where Ξ_ϵ is concentrated.
2. Our quasienergy E_ϵ may lie within the essential spectrum. In that case, one would expect a resonance near our quasienergy associated with the system being temporarily trapped in the well.
3. If $\inf\,(\sigma(h(y)) \setminus \mathcal{E}(y)) \,>\, 0$, $\;\liminf_{|y|\to\infty}\,\mathcal{E}(y) \,>\, 0$, and $\mathcal{E}$ has a unique global minimum at zero, then for small ϵ, the quasimode of the theorem is an exponentially accurate approximation to the $\alpha^{\rm th}$ eigenvalue of $H(\epsilon)$. This is proved by combining our results with those of [3].
4. The assumption that $\inf\,\sigma(h(y))$ is bounded below is just used to guarantee self–adjointness of $H(\epsilon)$. It never enters directly into our calculations, and it could be weakened.
5. Our estimates depend in complicated ways on various parameters of the problem. We have not kept track of the dependence of Λ and Γ on these parameters. We anticipate that doing so would be very tedious.

The time–independent Born–Oppenheimer approximation has a long history that dates back to [2]. The first mathematically rigorous result about its validity for low–lying states is [3], in which the expansion for the energy is proved to be accurate through fourth order in ϵ. Rigorous expansions to all orders are developed for systems with smooth potentials [4], diatomic Coulomb systems [5], and general Coulomb systems [13]. As we have already mentioned, the only previous construction of approximate solutions up to exponentially small errors is developed by the authors in [9].

Various other authors have studied time–independent Born–Oppenheimer limits for other problems. Sordoni [20] has extended the results mentioned above to include high angular momentum states of diatomic molecules. Herrin and Howland [10] have studied a situation in which the bundle of eigenvectors for the electron Hamiltonian had a non–trivial Berry phase. Rousse [19] has constructed quasimodes at fixed energies above the bottoms of wells when the nuclei have one degree of freedom. His results involved Bohr–Sommerfeld rules, and he handled level crossings and avoided crossings whose gaps had certain ϵ dependence. Klein, Martinez, and Messirdi [12, 14, 15, 17] have studied resonances whose lifetimes are finite because non–adiabatic transitions of the electrons coupled them to the continuous spectrum. In closely related subjects, we note rigorous exponentially accurate results for the time–dependent Born–Oppenheimer approximation [8, 16, 18] and for lifetimes of resonances [15, 17].

The paper is organized as follows: In Section 2, we derive the formal perturbation expansion that we use to prove Theorem 1. In Section 3, we study the growth of quantities that occur in the perturbation expansion. Then in Section 4, we prove the error bounds that imply Theorem 1.

2 The Perturbation Expansion

Our construction of the quasimodes involves the computation of formal Rayleigh–Schrödinger series in powers of ϵ, whose coefficients belong to the following Hilbert spaces:

1. The nuclear Hilbert space $L^2(\mathbb{R})$ (with Lebesgue measure), whose inner product and norm we denote respectively by $(\,\cdot,\cdot\,)$ and $\|\cdot\|$.
2. The electronic Hilbert space $\mathcal{H}_e$. The inner product and the norm we denote by $\langle\,\cdot,\,\cdot\,\rangle$ and $\|\cdot\|_e$.
3. The molecular Hilbert space $L^2(\mathbb{R},\mathcal{H}_e)$. The inner product is defined by
$$\int_{\mathbb{R}} \langle \Phi(x),\ \Psi(x)\rangle\, dx.$$
As already mentioned, we denote its norm by $|\!|\!|\cdot|\!|\!|$.

The operator $h(y)$ can be decomposed as

$$h(y) = \mathcal{E}(y)P(y) + h_\perp(y),$$

where $h_\perp(y) := h(y)(1-P(y))$ is an analytic family of type (A) in some neighborhood $S'' \subset S' \subset S$ around the origin. By shrinking S'' if necessary, we may assume that 0 belongs to the resolvent set of the restriction of $h_\perp(y)$ to the range of $(1 - P(y))$ for $y \in S''$. We let $h_\perp(0)^{-1}$ denote the reduced resolvent that is 0 in the range on $P(0)$. Henceforth, we assume that all the analytic properties used in the treatment of this problem are valid in the region S''.

After making the convenient scaling $y = \epsilon\, x$, the eigenvalue equation becomes

$$\left[-\frac{\epsilon^2}{2}\,\frac{d^2}{dx^2} \;+\; h(\epsilon x) \right]\; \Psi(\epsilon,\, x) \;=\; E(\epsilon)\; \Psi(\epsilon,\, x), \tag{1}$$

where $\Psi(\epsilon,\, x) \in L^2(\mathbb{R}, \mathcal{H}_e)$. With a slight abuse of notation, we henceforth denote the Hamiltonian operator in (1) by $H(\epsilon)$.

The function Ψ can be decomposed as

$$\Psi(\epsilon,\, x) \;=\; w(\epsilon,\, x)\; \Phi(\epsilon x) \;+\; \Psi_\perp(\epsilon,\, x),$$

where $\Phi(y)$ is the eigenvector associated to $\mathcal{E}(y)$ and $\langle \Phi(\epsilon x),\, \Psi_\perp(\epsilon, x)\rangle \;=\; 0$ for each x. We choose $\Phi(y)$ to be analytic for $y \in S''$ and normalized when $y \in S''$ is real. We choose its phase so that $\langle \Phi(y),\, \Phi'(y)\rangle = 0$. Since $\Psi_\perp(\epsilon,\, x) \;=\; (1 - P(\epsilon x))\;\; \Psi_\perp(\epsilon,\, x)$, the first and second derivatives of $\Psi(\epsilon,\, x)$ are given by

$$\begin{aligned}
\partial_x \Psi \;&=\; (\partial_x w)\,\Phi + \epsilon\, w\, \Phi' - \epsilon\, P'\, \Psi_\perp + (1-P)\; \partial_x \Psi_\perp, \qquad \text{and} \\
\partial_x^2 \Psi \;&=\; (\partial_x^2 w)\,\Phi + 2\,\epsilon\,(\partial_x w)\,\Phi' + \epsilon^2\, w\, \Phi'' - \epsilon^2\, P''\, \Psi_\perp - 2\,\epsilon\, P'\, \partial_x \Psi_\perp + (1-P)\; \partial_x^2 \Psi_\perp \\
\;&=\; \left(\partial_x^2 w + 2\,\epsilon\,\langle \Phi, \Phi'\rangle\, \partial_x w - 2\,\epsilon\,\langle \Phi, P'\partial_x \Psi_\perp\rangle + \epsilon^2\, w\,\langle \Phi, \Phi''\rangle - \epsilon^2\,\langle \Phi, P''\Psi_\perp\rangle \right) \Phi \\
&\quad +\; (1-P)\left(\partial_x^2 \Psi_\perp + 2\,\epsilon\,(\partial_x w)\,\Phi' - 2\,\epsilon\, P'\, \partial_x \Psi_\perp + \epsilon^2\, w\, \Phi'' - \epsilon^2\, P''\, \Psi_\perp \right).
\end{aligned}$$

Thus, in a neighborhood of 0, equation (1) is equivalent to the following pair of equations:

$$-\frac{\epsilon^2}{2}\, \partial_x^2 w - \epsilon^3\,\langle \Phi, \Phi'\rangle\, \partial_x w + \epsilon^3\,\langle \Phi, P'\partial_x \Psi_\perp\rangle - \frac{\epsilon^4}{2}\, w\,\langle \Phi, \Phi''\rangle + \frac{\epsilon^4}{2}\,\langle \Phi, P''\Psi_\perp\rangle + \mathcal{E} w \;=\; E w, \tag{2}$$

and

$$\begin{aligned}
-\frac{\epsilon^2}{2}&(1-P)\partial_x^2 \Psi_\perp - \epsilon^3 (\partial_x w)(1-P)\Phi' + \epsilon^3 (1-P)P'\partial_x \Psi_\perp \\
&- \frac{\epsilon^4}{2} w(1-P)\Phi'' + \frac{\epsilon^4}{2}(1-P)P''\Psi_\perp + h_\perp(1-P)\Psi_\perp \;=\; E(1-P)\Psi_\perp.
\end{aligned} \tag{3}$$

In order to take full advantage of the work done in [9], it is convenient to cast these equations in forms that resemble equations (3) and (4) of that paper. We first note that

$$\begin{aligned}
P \;&=\; \langle \Phi,\, \cdot\,\rangle\, \Phi, \\
P' \;&=\; \langle \Phi,\, \cdot\,\rangle\, \Phi' \;+\; \langle \Phi',\, \cdot\,\rangle\, \Phi, \\
P'' \;&=\; \langle \Phi,\, \cdot\,\rangle\, \Phi'' +\; 2\,\langle \Phi',\, \cdot\,\rangle\, \Phi' \;+\; \langle \Phi'',\, \cdot\,\rangle\, \Phi, \\
PP' \;&=\; \langle \Phi',\, \cdot\,\rangle\, \Phi, \quad \text{and} \\
PP'' \;&=\; \langle \Phi,\, \Phi''\rangle\, \langle \Phi,\, \cdot\,\rangle\, \Phi \;+\; \langle \Phi'',\, \cdot\,\rangle\, \Phi.
\end{aligned}$$

The last two identities follow from our phase condition $\langle \Phi,\, \Phi' \rangle = 0$ on Φ. It thus follows that $\langle \Phi',\, \Phi' \rangle = -\, \langle \Phi,\, \Phi'' \rangle = -\, \langle \Phi'',\, \Phi \rangle$. Also, from $\langle \Phi,\, \Psi_\perp \rangle = 0$, we easily obtain

$$\begin{aligned} \left\langle \Phi,\, \partial_x \Psi_\perp \right\rangle &= -\,\epsilon\, \langle \Phi',\, \Psi_\perp \rangle\,, \qquad \text{and} \\ \left\langle \Phi,\, \partial_x^2 \Psi_\perp \right\rangle &= -\,2\,\epsilon\, \langle \Phi',\, \partial_x \Psi_\perp \rangle \,+\, \epsilon^2\, \langle \Phi'',\, \Psi_\perp \rangle\,. \end{aligned}$$

With the use of these identities, equations (2) and (3) become

$$-\,\frac{\epsilon^2}{2} \partial_x^2 w \,+\, \epsilon^3\, \langle \Phi',\, \partial_x \Psi_\perp \rangle \,-\, \frac{\epsilon^4}{2}\, w\, \langle \Phi'',\, \Phi \rangle \,+\, \frac{\epsilon^4}{2}\, \langle \Phi'',\, \Psi_\perp \rangle \,+\, \mathcal{E}\, w \;=\; E\, w, \tag{4}$$

and

$$\begin{aligned} -\,\frac{\epsilon^2}{2}\, \partial_x^2 \Psi_\perp \,-\, \epsilon^3\, (\, \partial_x w\, \Phi' \,+\, \langle \Phi',\, \partial_x \Psi_\perp \rangle\; \Phi\,) & \\ -\,\frac{\epsilon^4}{2}\, w\, (\Phi'' - \langle \Phi,\, \Phi'' \rangle\, \Phi) \,-\, \frac{\epsilon^4}{2}\, \langle \Phi'',\, \Psi_\perp \rangle\; \Phi \,+\, h_\perp\, \Psi_\perp \;&=\; E\, \Psi_\perp. \end{aligned} \tag{5}$$

In order to simplify some expressions, we introduce the following notation:

$$\begin{aligned} \mathcal{A}(z) &= \Phi'(z), \\ \mathcal{B}(z) &= \langle \Phi''(z),\, \Phi(z) \rangle\,, \\ \mathcal{C}(z) &= \Phi''(z), \\ \mathcal{F}(z) &= \Phi''(z) \,-\, \langle \Phi(z),\, \Phi''(z) \rangle\; \Phi(z), \\ \mathcal{G}(z) &= \langle \Phi'(z),\, \cdot\, \rangle\; \Phi(z), \qquad \text{and} \\ \mathcal{K}(z) &= \langle \Phi''(z),\, \cdot\, \rangle\; \Phi(z). \end{aligned}$$

Note that $\mathcal{A}$, $\mathcal{C}$ and $\mathcal{F}$ are vector–valued functions, whereas $\mathcal{G}$ and $\mathcal{K}$ are operator–valued functions. All these functions are analytic in S''. Equations (4) and (5) can now be written as

$$-\,\frac{\epsilon^2}{2}\, \partial_x^2 w \,+\, \epsilon^3\, \langle \mathcal{A},\, \partial_x\, \Psi_\perp \rangle \,-\, \frac{\epsilon^4}{2}\, \mathcal{B}\, w \,+\, \frac{\epsilon^4}{2}\, \langle \mathcal{C},\, \Psi_\perp \rangle \,+\, \mathcal{E}\, w \;=\; E\, w, \tag{6}$$

and

$$-\,\frac{\epsilon^2}{2}\, \partial_x^2 \Psi_\perp \,-\, \epsilon^3\, (\, \partial_x w\, \mathcal{A} \,+\, \mathcal{G}\, \partial_x \Psi_\perp\,) \,-\, \frac{\epsilon^4}{2}\, w\, \mathcal{F} \,-\, \frac{\epsilon^4}{2}\, \mathcal{K}\, \Psi_\perp \,+\, h_\perp\, \Psi_\perp \;=\; E\, \Psi_\perp. \tag{7}$$

The functions defined above, along with $\mathcal{E}(z)$ and $\Phi(z)$, have convergent Taylor series in a neighborhood of 0. We denote these as

$$\mathcal{E}(\epsilon x) \;=\; \frac{1}{2}\, \epsilon^2\, x^2 \,+\, \sum_{n=3}^{\infty} d_n\, \epsilon^n\, x^n,$$

$$
\begin{aligned}
\Phi(\epsilon x) &= \sum_{n=0}^{\infty} \Phi_n\, \epsilon^n\, x^n, \\
\mathcal{A}(\epsilon x) &= \sum_{n=0}^{\infty} a_n\, \epsilon^n\, x^n, \\
\mathcal{B}(\epsilon x) &= \sum_{n=0}^{\infty} b_n\, \epsilon^n\, x^n, \\
\mathcal{C}(\epsilon x) &= \sum_{n=0}^{\infty} c_n\, \epsilon^n\, x^n, \\
\mathcal{F}(\epsilon x) &= \sum_{n=0}^{\infty} f_n\, \epsilon^n\, x^n, \\
\mathcal{G}(\epsilon x) &= \sum_{n=0}^{\infty} g_n\, \epsilon^n\, x^n, \qquad \text{and} \\
\mathcal{K}(\epsilon x) &= \sum_{n=0}^{\infty} k_n\, \epsilon^n\, x^n.
\end{aligned}
$$

The coefficients Φ_n, a_n, c_n, and f_n are vectors in $\mathcal{H}_e$. The coefficients g_n and k_n are bounded linear operators on $\mathcal{H}_e$ that satisfy the identities

$$
\begin{aligned}
g_n &= \sum_{p=0}^{n} \langle a_p,\, \cdot\, \rangle\, \Phi_{n-p}, \qquad \text{and} \\
k_n &= \sum_{p=0}^{n} \langle c_p,\, \cdot\, \rangle\, \Phi_{n-p}.
\end{aligned}
$$

A similar expansion can be performed on the (unbounded) operator–valued function $h_\perp(\epsilon x)$. Since $h_\perp$ is an analytic family in the sense of Kato, there exists a collection of operators $h_{\perp,n} : D \to \mathcal{H}_e$, all relatively bounded with respect to $h_{\perp,0} := h_\perp(0)$, such that

$$
h_\perp(\epsilon x)\, \Upsilon \;=\; \sum_{n=0}^{\infty} \epsilon^n\, x^n\, h_{\perp,n}\, \Upsilon
$$

in the strong sense, for every ϵx close to 0 and every $\Upsilon \in D$.

We now replace $E(\epsilon)$, $w(\epsilon, x)$ and $\Psi_\perp(\epsilon, x)$ by their formal Rayleigh–Schrödinger series,

$$
\begin{aligned}
E(\epsilon) &= \sum_{n=0}^{\infty} E_n\, \epsilon^n, \\
w(\epsilon,\, x) &= \sum_{n=0}^{\infty} w_n(x)\, \epsilon^n, \\
\Psi_\perp(\epsilon, x) &= \sum_{n=0}^{\infty} \Psi_{\perp,n}(x)\, \epsilon^n.
\end{aligned}
$$

We insert all these series into the equations (6) and (7) and equate terms of the same orders in ϵ on the two sides of the equations. This yields the following:

Order 0:

$$E_0\, w_0 \;=\; 0, \qquad \text{and}$$
$$h_{\perp,0}\, \Psi_{\perp,0} \;=\; E_0\, \Psi_{\perp,0}.$$

Since we want $w_0 \neq 0$, the first equation requires $E_0 = 0$. Since $0 \notin \sigma\,(h_{\perp,0})$, the second equation forces $\Psi_{\perp,0} = 0$.

Order 1:

$$E_0\, w_1 \;+\; E_1\, w_0 \;=\; 0, \qquad \text{and}$$
$$h_{\perp,0}\, \Psi_{\perp,1} \;+\; x\, h_{\perp,1}\, \Psi_{\perp,0} \;=\; E_0\, \Psi_{\perp,1} \;+\; E_1\, \Psi_{\perp,0}.$$

The first equation requires $E_1 = 0$. The second equation then forces $\Psi_{\perp,1} = 0$.

Order 2:

$$-\,\frac{1}{2}\,\partial_x^2\, w_0 \;+\; \frac{1}{2}\,x^2\, w_0 \;=\; E_2\, w_0, \qquad \text{and}$$
$$h_{\perp,0}\, \Psi_{\perp,2} \;=\; 0.$$

Clearly E_2 and w_0 must be solutions to the eigenvalue problem for the harmonic oscillator Hamiltonian

$$H_0 \;=\; -\,\frac{1}{2}\,\frac{d^2}{dx^2} \;+\; \frac{1}{2}\,x^2,$$

whose eigenvalues and normalized eigenfunctions are $(\alpha+1/2)$ and $\phi_\alpha(x)$, where $\alpha = 0, 1, 2, 3, \ldots$ We fix a choice of α and then have $E_2 = (\alpha+1/2)$, and $w_0 = \phi_\alpha$. The second equation requires $\Psi_{\perp,2} = 0$.

Order 3:

$$(H_0 - E_2)\, w_1 \;+\; \langle a_0,\, \partial_x \Psi_{\perp,0} \rangle \;+\; d_3\, x^3\, w_0 \;=\; E_3\, w_0, \qquad \text{and}$$
$$-\;(\partial_x w_0)\;a_0 \;+\; h_{\perp,0}\, \Psi_{\perp,3} \;=\; 0.$$

Equating components in the direction of ϕ_α in the first equation leads to $E_3 = 0$. The orthogonal components then require

$$w_1 \;=\; -\,d_3\,(H_0 - E_2)_\perp^{-1}\, x^3\, w_0,$$

where $(H_0 - E_2)_\perp^{-1}$ denotes the inverse of the restriction of $(H_0 - E_2)$ to the subspace orthogonal to ϕ_α. We henceforth arbitrarily assume that $w_n \perp \phi_\alpha$ for all $n > 0$. The second equation yields

$$\Psi_{\perp,3} \;=\; (\partial_x w_0)\;(h_{\perp,0})^{-1}\, a_0.$$

Remark In the Order 3 calculations, E_3 vanishes because $(\,\phi_\alpha,\, x^3\,\phi_\alpha\,)\;=\;0$. The symmetry that forces this inner product to vanish also causes $E_n=0$ for all odd values of n in the higher order calculations. We do not make use of this fact in our estimates.

Order $\mathbf{n\geq 4}$:

$$\begin{aligned}(H_0-E_2)\,w_{n-2}\;+\;&\sum_{m=0}^{n-3}\,x^m\;\langle a_m,\,\partial_x\,\Psi_{\perp,n-m-3}\rangle-\;\frac{1}{2}\,\sum_{m=0}^{n-4}\,b_m\,x^m\,w_{n-m-4}\\ &+\frac{1}{2}\sum_{m=0}^{n-4}\,x^m\;\langle c_m,\,\Psi_{\perp,n-m-4}\rangle\;+\;\sum_{m=3}^{n}\,d_m\,x^m\,w_{n-m}\quad=\quad\sum_{m=2}^{n}\,E_m\,w_{n-m},\end{aligned}$$

and

$$\begin{aligned}-\,\frac{1}{2}\,\partial_x^2\,\Psi_{\perp,n-2}\;-\;\sum_{m=0}^{n-3}a_m\,x^m\,\partial_x w_{n-m-3}\;-\;\sum_{m=0}^{n-3}g_m\,x^m\,\partial_x\Psi_{\perp,n-3-m}\;-\;\frac{1}{2}\sum_{m=0}^{n-4}f_m\,x^m\,w_{n-m-4}\\ -\,\frac{1}{2}\,\sum_{m=0}^{n-4}\,x^m\,k_m\,\Psi_{\perp,n-4-m}+\sum_{m=0}^{n}\,x^m\,h_{\perp,m}\,\Psi_{\perp,n-m}\quad=\quad\sum_{m=2}^{n}\,E_m\,\Psi_{\perp,n-m}.\end{aligned}$$

We now project the two sides of the first equation into the ϕ_α direction to obtain a formula for E_n. Then projecting onto the subspace orthogonal to ϕ_α, we obtain an equation for $(H_0-E_2)\,w_{n-2}$. We determine w_{n-2} by applying the reduced resolvent $(H_0-E_2)_\perp^{-1}$. We then solve the second equation for $\Psi_{\perp,n}$ by applying the reduced resolvent $(h_{\perp,0})^{-1}$ to both sides of that equation. We therefore have, for $n\geq 4$,

$$\begin{aligned}E_n\;&=\;\sum_{m=0}^{n-6}\,(\phi_\alpha,\,x^m\,\langle a_m,\,\partial_x\,\Psi_{\perp,n-m-3}\rangle)\;-\;\frac{1}{2}\,\sum_{m=0}^{n-4}\,b_m\,(\phi_\alpha,\,x^m\,w_{n-m-4})\\ &\quad+\,\frac{1}{2}\,\sum_{m=0}^{n-7}\,(\phi_\alpha,\,x^m\,\langle c_m,\,\Psi_{\perp,n-m-4}\rangle)\;+\;\sum_{m=3}^{n}\,d_m\,(\phi_\alpha,\,x^m\,w_{n-m})\,,\end{aligned}$$

$$\begin{aligned}w_{n-2}\;&=\;(H_0-E_2)_\perp^{-1}\,\Bigg[\,-\sum_{m=0}^{n-6}\,x^m\,\langle a_m,\,\partial_x\,\Psi_{\perp,n-m-3}\rangle\;+\;\frac{1}{2}\,\sum_{m=0}^{n-4}\,b_m\,x^m\,w_{n-m-4}\\ &\qquad-\,\frac{1}{2}\sum_{m=0}^{n-7}\,x^m\,\langle c_m,\,\Psi_{\perp,n-m-4}\rangle\;-\;\sum_{m=0}^{n}\,d_m\,x^m\,w_{n-m}\;+\;\sum_{m=2}^{n}\,E_m\,w_{n-m}\,\Bigg],\end{aligned}$$

and

$$\Psi_{\perp,n}\;=\;(h_{\perp,0})^{-1}\,\Bigg[\,\frac{1}{2}\,\partial_x^2\,\Psi_{\perp,n-2}\;+\;\sum_{m=0}^{n-3}\,a_m\,x^m\,\partial_x\,w_{n-m-3}\;+\;\sum_{m=0}^{n-6}\,x^m\,g_m\,\partial_x\,\Psi_{\perp,n-3-m}$$

$$
- \frac{1}{2} \sum_{m=0}^{n-4} f_m \, x^m \, w_{n-m-4} \; - \; \frac{1}{2} \sum_{m=0}^{n-7} x^m \, k_m \, \Psi_{\perp,n-4-m}
$$

$$
+ \sum_{m=1}^{n-3} x^m \, h_{\perp,m} \Psi_{\perp,n-m} \; + \; \sum_{m=2}^{n-3} E_m \, \Psi_{\perp,n-m} \Bigg] .
$$

In the sequel, we use the fact that $L^2(\mathbb{R}, \mathcal{H}_e)$ is isomorphic to $L^2(\mathbb{R}) \otimes \mathcal{H}_e$. Let $U : L^2(\mathbb{R}) \otimes \mathcal{H}_e \to L^2(\mathbb{R}, \mathcal{H}_e)$ denote the natural isomorphism defined by

$$
U(\phi(x) \otimes \Upsilon) = \phi(x) \Upsilon .
$$

Although the set of recursive equations given above involves certain unbounded operators, they can be reduced to bounded operators because of the following result.

Lemma 1 *Let $P_{i \leq n}$ denote the projection onto the span of ϕ_i's with $0 \leq i \leq n$. Then*

$$
\begin{aligned}
& w_n \in Ran\,(P_{i \leq 3n+\alpha}) && \textit{for all} \quad n \geq 0, \\
& \Psi_{\perp,n} \in Ran\,(U\,(P_{i \leq 3n+\alpha-8} \otimes I)\,U^\star) && \textit{for all} \quad n \geq 3.
\end{aligned}
$$

Proof: We prove this by an easy induction using the equations that define w_{n-2} and Ψ_n. □

In order to obtain estimates that are sharp enough for our purposes, we transform the problem, using a method originally developed in [21, 22]. We introduce a bounded operator A, which depends on the choice of α, by defining its action on the basis of the harmonic oscillator Hamiltonian:

$$
A\,\phi_\beta \; = \; \begin{cases} \phi_\beta & \text{if} \quad \beta = \alpha, \\ |\beta - \alpha|^{-1/2}\,\phi_\beta & \text{if} \quad \beta \neq \alpha. \end{cases}
$$

We then define $\tilde{A} : L^2(\mathbb{R}, \mathcal{H}_e) \to L^2(\mathbb{R}, \mathcal{H}_e)$ as $\tilde{A} = U(A \otimes I)U^\star$. These operators satisfy the following identity.

Lemma 2 *Consider any $\Psi(x) \in L^2(\mathbb{R}, \mathcal{H}_e)$ and $\Theta \in \mathcal{H}_e$. Then,*

$$
\langle \Theta,\, U(A \otimes I)U^\star \Psi(x) \rangle \; = \; A\,\langle \Theta,\, \Psi(x) \rangle \, .
$$

As a consequence, the operators g_m and k_m all commute with $\tilde{A}$.

Proof: Let $\{\Upsilon_m\}$ be a basis of $\mathcal{H}_e$ and $\{\phi_\alpha(x)\}$ a basis of $L^2(\mathbb{R})$. Then $\{\phi_\alpha(x)\Upsilon_m\}$ is a basis of $L^2(\mathbb{R}, \mathcal{H}_e)$ and

$$
\langle \Theta,\, U(A \otimes I)U^\star(\phi_\alpha(x)\Upsilon_m) \rangle \;\; = \;\; \langle \Theta,\, U(A \otimes I)(\phi_\alpha(x) \otimes \Upsilon_m) \rangle
$$

$$
\begin{aligned}
&= \langle \Theta,\, U((A\phi_\alpha)(x) \otimes \Upsilon_m)\rangle \\
&= \langle \Theta,\, (A\phi_\alpha)(x)\Upsilon_m\rangle \\
&= (A\phi_\alpha)(x)\, \langle \Theta,\, \Upsilon_m\rangle \\
&= A\,\langle \Theta,\, \phi_\alpha(x)\Upsilon_m\rangle\,.
\end{aligned}
$$

Now extend by linearity. □

Rather than estimating the norms of w_n and $\Psi_{\perp,n}$ directly, we study $\hat{w}_n$ and $\hat{\Psi}_{\perp,n}$, where $w_n = A\,\hat{w}_n$ and $\Psi_{\perp,n} = h_{\perp,0}^{-1}\,\tilde{A}\,\hat{\Psi}_{\perp,n} = \tilde{A}\,h_{\perp,0}^{-1}\,\hat{\Psi}_{\perp,n}$. These definitions make sense because all finite linear combinations of ϕ_i's are in the domain of the unbounded operator A^{-1}. We define $\tilde{A}^{-1} = U(A^{-1} \otimes I)U^{\star}$. In addition, we multiply (6) and (7) by A and $\tilde{A}$ respectively. Afterward we use Lemma 2. In this manner we obtain the following:

$$
\begin{aligned}
E_0 &= E_1 = E_3 = 0, \\
E_2 &= \alpha + 1/2, \\
\hat{w}_0 &= \phi_\alpha, \\
\hat{w}_1 &= -\,d_3\,[A(H_0 - E_2)A]_\perp^{-1}\,A\,x^3\,A\,\hat{w}_0, \\
\hat{\Psi}_{\perp,0} &= \hat{\Psi}_{\perp,1} = \hat{\Psi}_{\perp,2} = 0, \\
\hat{\Psi}_{\perp,3} &= \tilde{A}^{-1}\,(\partial_x w_0)\,a_0,
\end{aligned}
$$

and for $n \geq 4$,

$$
\begin{aligned}
E_n &= \sum_{m=0}^{n-6} \Big(A\,\partial_x\,x^m\,A\,\phi_\alpha,\, \Big\langle a_m,\; h_{\perp,0}^{-1}\,\hat{\Psi}_{\perp,n-m-3}\Big\rangle\Big) \;-\; \frac{1}{2}\sum_{m=0}^{n-4} b_m\,(A\,x^m\,A\,\phi_\alpha,\, \hat{w}_{n-m-4}) \\
&\quad + \frac{1}{2}\sum_{m=0}^{n-7} \Big(A\,x^m\,A\,\phi_\alpha,\, \Big\langle c_m,\; h_{\perp,0}^{-1}\,\hat{\Psi}_{\perp,n-m-4}\Big\rangle\Big) \;+\; \sum_{m=3}^{n} d_m\,(A\,x^m\,A\,\phi_\alpha,\, \hat{w}_{n-m})\,,
\end{aligned}
$$

$$
\begin{aligned}
\hat{w}_{n-2} &= [A(H_0 - E_2)A]_\perp^{-1}\Bigg[-\sum_{m=0}^{n-6} A\,x^m\,\partial_x\,A\Big\langle a_m,\, h_{\perp,0}^{-1}\,\hat{\Psi}_{\perp,n-m-3}\Big\rangle + \frac{1}{2}\sum_{m=0}^{n-4} b_m\,A\,x^m A\,\hat{w}_{n-m-4} \\
&\qquad - \frac{1}{2}\sum_{m=0}^{n-7} A\,x^m\,A\Big\langle c_m,\, h_{\perp,0}^{-1}\,\hat{\Psi}_{\perp,n-m-4}\Big\rangle \;-\; \sum_{m=3}^{n} d_m\,A\,x^m A\,\hat{w}_{n-m} \\
&\qquad + \sum_{m=2}^{n} E_m\,A^2\,\hat{w}_{n-m}\Bigg],
\end{aligned}
$$

and

$$
\begin{aligned}
\hat{\Psi}_{\perp,n} \;=\; \tilde{A}^{-1} \Bigg[& \frac{1}{2}\,\partial_x^2\,\tilde{A}\,h_{\perp,0}^{-1}\,\hat{\Psi}_{\perp,n-2} \;+\; \sum_{m=0}^{n-3} a_m\,x^m\,\partial_x\,A\,\hat{w}_{n-m-3} \\
& + \sum_{m=0}^{n-6} x^m\,\partial_x\,\tilde{A}\,g_m\,h_{\perp,0}^{-1}\,\hat{\Psi}_{\perp,n-3-m} \;-\; \frac{1}{2}\sum_{m=0}^{n-4} f_m\,x^m\,A\,\hat{w}_{n-m-4} \\
& - \frac{1}{2}\sum_{m=0}^{n-7} x^m\,\tilde{A}\,k_m\,h_{\perp,0}^{-1}\,\hat{\Psi}_{\perp,n-4-m} \;+\; \sum_{m=1}^{n-3} x^m\,h_{\perp,m}\,\tilde{A}\,h_{\perp,0}^{-1}\,\hat{\Psi}_{\perp,n-m} \\
& + \sum_{m=2}^{n-3} E_m\,\tilde{A}\,h_{\perp,0}^{-1}\,\hat{\Psi}_{\perp,n-m} \Bigg].
\end{aligned}
$$

3 Growth of the Perturbation Coefficients

In this section we obtain nice upper bounds for the growth of the norms of $|E_n|$, $\|\hat{w}_{n-2}\|$ and $|||\hat{\Psi}_n|||$. We do this by first getting recursive inequalities for $|E_n|$, $\|\hat{w}_{n-2}\|$ and $|||\hat{\Psi}_n|||$ from the equations described in the previous section. Then an induction argument yields the desired estimates.

Let us first note that the region S'' contains the complex disc of radius δ centered at the origin. Since certain functions involved in this problem are analytic in S'', we can use the Cauchy integral formula to conclude that $\|\Phi_m\|_e$, $\|a_m\|_e$, $|b_m|$, $\|c_m\|_e$, $\|f_m\|_e$, and $|d_m|$ are all bounded by $Z\,\delta^{-m}$, for some constant $Z>0$. Also, $\|g_m\|_e$ and $\|k_m\|_e$ are bounded by $(m+1)\,Z^2\,\delta^{-m}$. Furthermore, various operators that show up in the last three equations of Section 2 satisfy some of the following statements.

Lemma 3 *Let $\#_x$ denote either x or ∂_x, and let $(\#_x)^l$ denote any product of l factors, each of which is either x or ∂_x. Then*

1. *The operators $h_{\perp,m}$ and $h_{\perp,0}^{-1}$ conmute with the operators $\tilde{A}$, $\tilde{A}^{-1}$ and $(\#_x)^l$.*

2. $\left|\left|\left|\tilde{A}^{-1}\,(\#_x)^l\,\tilde{A}\,U\,(P_{i\leq n}\otimes I)\,U^\star\right|\right|\right| = \left\|A^{-1}\,(\#_x)^l\,A\,P_{i\leq n}\right\|.$

Also,

3. *The operators $h_{\perp,m}\,h_{\perp,0}^{-1}:\mathcal{H}_e\to\mathcal{H}_e$ satisfy $\left\|h_{\perp,m}\,h_{\perp,0}^{-1}\right\|_e\leq Z\,\delta^{-m}$, where Z is the constant introduced above, properly redefined if necessary.*

Proof: 1. This result follows since $h_{\perp,m}$ and $h_{\perp,0}^{-1}$ act in the electron variables, while x and ∂_x act in the nuclear variables.

2. This result is a consequence of the electronic variables playing no significant role in the operators involved.
3. We have assumed that $h(\cdot)$ is an analytic family of type (A) with domain D. By results of Section 2 of Chapter 7 of [11], it follows that $h(y)\, h_{\perp,0}^{-1}$ is a bounded analytic family on $\mathcal{H}_e$. The Taylor series coefficients of this operator valued function are $h_{\perp,m}\, h_{\perp,0}^{-1}$, and the radius of convergence is at least δ. The result follows from the standard Cauchy estimates. $\square$

Using Lemmas 1 and 3 we obtain the following set of inequalities:

$$\begin{aligned}
|E_n| \;&\le\; Z \sum_{m=0}^{n-6} \delta^{-m} \|A\,\partial_x\, x^m A\, P_{i\le\alpha}\| \left\|\left|\hat{\Psi}_{\perp,n-m-3}\right\|\right| \;+\; \frac{Z}{2} \sum_{m=0}^{n-4} \delta^{-m} \|A\, x^m A\, P_{i\le\alpha}\| \|\hat{w}_{n-m-4}\| \\
&\quad + \frac{Z}{2} \sum_{m=0}^{n-7} \delta^{-m} \|\, A\, x^m A\, P_{i\le\alpha}\| \left\|\left|\hat{\Psi}_{\perp,n-m-4}\right\|\right| \;+\; Z \sum_{m=3}^{n} \delta^{-m} \|A\, x^m A\, P_{i\le\alpha}\| \|\hat{w}_{n-m}\|\,,
\end{aligned}$$

$$\begin{aligned}
\|\hat{w}_{n-2}\| \;&\le\; Z \sum_{m=0}^{n-6} \delta^{-m} \|A\,\partial_x\, x^m A\, P_{i\le 3(n-m-3)+\alpha-8}\| \left\|\left|\hat{\Psi}_{\perp,n-m-3}\right\|\right| \\
&\quad + \frac{Z}{2} \sum_{m=0}^{n-4} \delta^{-m} \|A\, x^m A\, P_{i\le 3(n-m-4)+\alpha}\| \|\hat{w}_{n-m-4}\| \\
&\quad + \frac{Z}{2} \sum_{m=0}^{n-7} \delta^{-m} \|\, A\, x^m A\, P_{i\le 3(n-m-4)+\alpha-8}\| \left\|\left|\hat{\Psi}_{\perp,n-m-4}\right\|\right| \\
&\quad + Z \sum_{m=3}^{n} \delta^{-m} \|A\, x^m A\, P_{i\le 3(n-m)+\alpha}\| \|\hat{w}_{n-m}\| \;+\; \sum_{m=2}^{n} |E_m| \|\hat{w}_{n-m}\|\,,
\end{aligned}$$

and

$$\begin{aligned}
\left\|\left|\hat{\Psi}_{\perp,n}\right\|\right| \;&\le\; \frac{\left\|h_{\perp,0}^{-1}\right\|_e}{2} \left\|A^{-1}\, \partial_x^2\, \tilde{A}\, P_{i\le 3(n-2)+\alpha-8}\right\| \left\|\left|\hat{\Psi}_{\perp,n-2}\right\|\right| \\
&\quad + Z \sum_{m=0}^{n-3} \delta^{-m} \left\|A^{-1}\, x^m\, \partial_x\, A\, P_{i\le 3(n-m-3)+\alpha}\right\| \|\hat{w}_{n-m-3}\| \\
&\quad + Z^2 \left\|h_{\perp,0}^{-1}\right\|_e \sum_{m=0}^{n-6} \delta^{-m}\, (m+1) \left\|A^{-1}\, x^m\, \partial_x\, A\, P_{i\le 3(n-m-3)+\alpha-8}\right\| \left\|\left|\hat{\Psi}_{\perp,n-m-3}\right\|\right| \\
&\quad + \frac{Z}{2} \sum_{m=0}^{n-4} \delta^{-m} \left\|A^{-1}\, x^m\, A\, P_{i\le 3(n-m-4)+\alpha}\right\| \|\hat{w}_{n-m-4}\|
\end{aligned}$$

$$+ \frac{Z^2 \left\|h_{\perp,0}^{-1}\right\|_e}{2} \sum_{m=0}^{n-7} \delta^{-m} \, (m+1) \left\| A^{-1} \, x^m \, A \, P_{i \leq 3(n-m-4)+\alpha-8} \right\| \left|\left|\left| \hat{\Psi}_{\perp,n-m-4} \right|\right|\right|$$

$$+ \, Z \sum_{m=1}^{n} \delta^{-m} \left\| A^{-1} \, x^m \, A \, P_{i \leq 3(n-m)+\alpha-8} \right\| \left|\left|\left| \hat{\Psi}_{\perp,n-m} \right|\right|\right|$$

$$+ \, \left\|h_{\perp,0}^{-1}\right\|_e \sum_{m=0}^{n} |E_m| \left|\left|\left| \hat{\Psi}_{\perp,n-m} \right|\right|\right| \, .$$

These inequalities differ only in unimportant ways from those preceding (16) in [9]. This leads us to the following result.

Theorem 2 *Define $\kappa := 2/\delta^2$. There exists $b > 1$ such that for every $n \geq 3$ we have*

$$\begin{aligned} |E_n| &< \kappa^{3(n-2)} \, b^{2n-5} \, [(n+\alpha-2)!]^{1/2}, \\ \|\hat{w}_{n-2}\| &< \kappa^{3(n-2)} \, b^{2n-3} \, [(n+\alpha-1)!]^{1/2}, \qquad \textit{and} \\ \left|\left|\left| \hat{\Psi}_{\perp,n} \right|\right|\right| &< \kappa^{3n} \, b^{2n-1} \, [(n+\alpha-1)!]^{1/2}. \end{aligned}$$

The rather tedious proof of this theorem is based on a simple induction argument. We refer to the proof of Theorem 2 of [9] for the details.

4 Estimates for the Norm of the Error

The construction of the exponentially accurate quasimodes is based on truncation of the formal Rayleigh–Schrödinger series whose coefficients obey the growth estimates stated in Theorem 2. Here we mimic to a certain extent the arguments in [21, 22], which are based on a technique developed in [7]. The main change in our present case is that the recursion relations that generate these coefficients make sense only in a neighborhood of the bottom of the energy surface $\mathcal{E}(y)$. This issue will be dealt with by using a suitable cut–off function. In order to prove certain estimates, we henceforth assume that the region $S'' \subset \mathbb{C}$ contains the open set

$$\{z \in \mathbb{C} : |z+s| < \delta+\mu\} \cup \{z \in \mathbb{C} : |z-s| < \delta+\mu\} \cup \{z \in \mathbb{C} : |\mathrm{Re}\, z| < s \ , \ |\mathrm{Im}\, z| < \delta+\mu\},$$

for some fixed $s > 0$, $1 \geq \delta > 0$ and $\mu > 0$ arbitrarily small.

For $N \geq 1$ define

$$E^N \;\; := \;\; \sum_{n=0}^{N+2} \epsilon^n \, E_n,$$

$$
\begin{aligned}
w^N(\epsilon,x) &:= \sum_{n=0}^{N} \epsilon^n \, w_n(\epsilon,x), \\
\Psi_\perp^N(\epsilon,x) &:= \sum_{n=0}^{N+2} \epsilon^n \, \Psi_{\perp,n}(\epsilon,x), \qquad \text{and} \\
\Psi^N(\epsilon,x) &:= w^N(\epsilon,x)\,\Phi(\epsilon x) \;+\; \Psi_\perp^N(\epsilon,x).
\end{aligned}
$$

Let f be a real C^2 function, such that $f(y) = 1$ for $y \in [-r/\epsilon, r/\epsilon]$ and $f(y) = 0$ for $y \notin [-s/\epsilon, s/\epsilon]$, where $s > r > 0$. The support of f' is then contained in $[-s/\epsilon, -r/\epsilon] \cup [r/\epsilon, s/\epsilon]$. For later use, let $\chi_{f'}$ denote the characteristic function of the support of f'.

We now define

$$
\Xi^N(\epsilon,x) \;:=\; f(x)\,\Psi^N(\epsilon,x).
$$

Let $H(\epsilon)$ denote the self–adjoint operator defined in equation (1). The error commited when truncated Rayleigh–Schrödinger series replace the actual solution to equation (1) is given by

$$
\left(H(\epsilon) - E^N\right)\Xi^N \;=\; f\left(H(\epsilon) - E^N\right)\Psi^N - \frac{\epsilon^2}{2}\left[\partial_x^2, f\right]\Psi^N. \tag{8}
$$

The first term can be written as (temporarily ignoring the cut–off)

$$
\left(H(\epsilon) - E^N\right)\Psi^N \;=\; S_N\,\Phi \;+\; T_N,
$$

where the residual terms S_N and T_N are given explicitly by

$$
\begin{aligned}
S_N \;&:=\; -\frac{\epsilon^2}{2}\,\partial_x^2\, w^N + \epsilon^3\left\langle \mathcal{A},\, \partial_x\,\Psi_\perp^N\right\rangle - \frac{\epsilon^4}{2}\,\mathcal{B}\,w^N + \frac{\epsilon^4}{2}\,\left\langle \mathcal{C},\, \Psi_\perp^N\right\rangle + \mathcal{E}\,w^N \;-\; E^N\,w^N, \quad \text{and} \\
T_N \;&:=\; -\frac{\epsilon^2}{2}\,\partial_x^2\,\Psi_\perp^N \;-\; \epsilon^3\left(\partial_x\,w^N\,\mathcal{A} \;+\; \mathcal{G}\,\partial_x\,\Psi_\perp^N\right) \;-\; \frac{\epsilon^4}{2}\,w^N\,\mathcal{F} \;-\; \frac{\epsilon^4}{2}\,\mathcal{K}\,\Psi_\perp^N \\
&\qquad +h_\perp\Psi_\perp^N \;-\; E^N\,\Psi_\perp^N.
\end{aligned}
$$

Since the perturbation coefficients are the solutions to the recursive equations obtained in Section 2, all terms of order $n \le N+2$ cancel in both S_N and T_N. Thus, the residual terms can be written as

$$
\begin{aligned}
S_N \;=\; &\sum_{m=0}^{N} \epsilon^{m+3}\left\langle \mathcal{A}^{[N-m-1]},\, \partial_x\Psi_{\perp,m}\right\rangle \;+\; \epsilon^{N+4}\left\langle \mathcal{A}^{[-1]},\, \partial_x\Psi_{\perp,N+1}\right\rangle \;+\; \epsilon^{N+5}\left\langle \mathcal{A}^{[-1]},\, \partial_x\Psi_{\perp,N+2}\right\rangle \\
&-\frac{1}{2}\sum_{m=0}^{N-1} \epsilon^{m+4}\,\mathcal{B}^{[N-m-2]}\,w_m \;-\; \frac{\epsilon^{N+4}}{2}\,\mathcal{B}^{[-1]}\,w_N \\
&+\frac{1}{2}\sum_{m=0}^{N-1} \epsilon^{m+4}\left\langle \mathcal{C}^{[N-m-2]},\; \Psi_{\perp,m}\right\rangle
\end{aligned}
$$

$$
\begin{aligned}
&+ \frac{\epsilon^{N+4}}{2} \left\langle \mathcal{C}^{[-1]},\, \Psi_{\perp,N} \right\rangle \,+\, \frac{\epsilon^{N+5}}{2} \left\langle \mathcal{C}^{[-1]},\, \Psi_{\perp,N+1} \right\rangle \,+\, \frac{\epsilon^{N+6}}{2} \left\langle \mathcal{C}^{[-1]},\, \Psi_{\perp,N+2} \right\rangle \\
&+ \sum_{m=0}^{N} \epsilon^m \, \mathcal{E}^{[N-m+2]} \, w_m \\
&- \sum_{l=N+3}^{2N+2} \epsilon^l \sum_{m=l-N-2}^{N} E_{l-m} \, w_m \,,
\end{aligned}
$$

and

$$
\begin{aligned}
T_N \;=\; & -\frac{1}{2} \, \epsilon^{N+3} \, \partial_x^2 \, \Psi_{\perp,N+1} \,-\, \frac{1}{2} \, \epsilon^{N+4} \, \partial_x^2 \, \Psi_{\perp,N+2} \\
& - \sum_{m=0}^{N} \epsilon^{m+3} \, (\partial_x \, w_m) \, \mathcal{A}^{[N-m-1]} \\
& - \sum_{m=0}^{N} \epsilon^{m+3} \, \mathcal{G}^{[N-m-1]} \, \partial_x \, \Psi_{\perp,m} \,-\, \epsilon^{N+4} \, \mathcal{G}^{[-1]} \, \partial_x \, \Psi_{\perp,N+1} \,-\, \epsilon^{N+5} \, \mathcal{G}^{[-1]} \, \partial_x \, \Psi_{\perp,N+2} \\
& - \frac{1}{2} \sum_{m=0}^{N-1} \epsilon^{m+4} \, \mathcal{F}^{[N-m-2]} \, w_m \,-\, \frac{\epsilon^{N+4}}{2} \, \mathcal{F}^{[-1]} \, w_N \\
& - \frac{1}{2} \sum_{m=0}^{N-1} \epsilon^{m+4} \, \mathcal{K}^{[N-m-2]} \, \Psi_{\perp,m} \\
& - \frac{\epsilon^{N+4}}{2} \, \mathcal{K}^{[-1]} \, \Psi_{\perp,N} \,-\, \frac{\epsilon^{N+5}}{2} \, \mathcal{K}^{[-1]} \, \Psi_{\perp,N+1} \,-\, \frac{\epsilon^{N+6}}{2} \, \mathcal{K}^{[-1]} \, \Psi_{\perp,N+2} \\
& + \sum_{m=0}^{N+2} \epsilon^m \, h_{\perp}^{[N-m+2]} \, \Psi_{\perp,m} \\
& - \sum_{l=N+3}^{2N+4} \epsilon^l \sum_{m=l-N-2}^{N+2} E_{l-m} \, \Psi_{\perp,m} \,.
\end{aligned}
$$

We have used above the following notation for exact Taylor series errors for any function $g(z)$ expanded around $z = 0$:

$$
g^{[n]}(z) \;:=\; \begin{cases} g(z) \;-\; \displaystyle\sum_{m=0}^{n} \frac{g^{(m)}}{m!} \, z^m & \text{if} \quad n \geq 0, \\[2ex] \qquad\quad g(z) & \text{if} \quad n = -1. \end{cases}
$$

Note that in this notation, the integer n may never be less than -1, and that $g^{[n]}$ is $O(\epsilon^{n+1})$

since $z = \epsilon\, x$. Similarly,

$$h_\perp^{[n]}(z)\ \Upsilon\ \ :=\ \begin{cases} h_\perp(z)\ \Upsilon\ -\ \displaystyle\sum_{m=0}^{n}\ z^m\, h_{\perp,m}\ \Upsilon & \text{if}\quad n \geq 0, \\[2ex] \qquad h_\perp(z)\ \Upsilon & \text{if}\quad n = -1, \end{cases}$$

for every $\Upsilon \in D$.

Our main result in this work relies on an upper bound for the $L^2(\mathbb{R}, \mathcal{H}_e)$-norm of (8). We obviously have

$$\begin{aligned} \left\| \left(H(\epsilon) - E^N\right) \Xi^N \right\| \ &\leq\ \left\| f\, \left(H(\epsilon) - E^N\right) \Psi^N \right\|\ +\ \frac{\epsilon^2}{2}\, \left\| \left[\partial_x^2, f\right]\, \Psi^N \right\| \\ &\leq\ \| f\, S_N\, \Phi \|\ +\ \| f\, T_N \|\ +\ \frac{\epsilon^2}{2}\, \left\| \left[\partial_x^2, f\right]\, \Psi^N \right\| \\ &\leq\ \| f\, S_N \|\ +\ \| f\, T_N \|\ +\ \frac{\epsilon^2}{2}\, \left\| \left[\partial_x^2, f\right]\, \Psi^N \right\| \end{aligned} \tag{9}$$

We use the following three propositions to estimate the last line in this expression.

Proposition 1 *There exist constants G_1 and F_1, such that*

$$\| f\, S_N \|\ <\ \sum_{m=N+3}^{2N+2}\ G_1\, F_1^m\, \epsilon^m\, [(m + \alpha + 1)!]^{1/2},$$

for every $\epsilon > 0$.

Proposition 2 *There exist constants G_2 and F_2, such that*

$$\| f\, T_N \|\ <\ \sum_{m=N+3}^{2N+2}\ G_2\, F_2^m\, \epsilon^m\, [(m + \alpha + 1)!]^{1/2},$$

for every $\epsilon > 0$.

For the third proposition, we introduce $\hat{\Psi}^N$, which is defined as

$$\hat{\Psi}^N(\epsilon, x)\ :=\ \hat{w}^N(\epsilon, x)\, \Phi(\epsilon x)\ +\ \hat{\Psi}_\perp^N(\epsilon, x).$$

Here $\hat{w}^N$ and $\hat{\Psi}_\perp^N$ are given by $w^N = A\, \hat{w}^N$ and $\Psi_\perp^N = h_{\perp,0}^{-1}\, \tilde{A}\, \hat{\Psi}_\perp^N$.

Proposition 3 *Let r and s be the numbers that define the support of f'. Then, for every $\epsilon > 0$ that satisfies $r^2/\epsilon^2 \geq 6N + 2\alpha + 3$, we have*

$$\left\| \left[\partial_x^2, f \right] \Psi^N \right\| \;<\; G_0(\epsilon)\; 2^{3N+\alpha}\; \frac{\exp\left(-\frac{r^2}{2\epsilon^2}\right)}{\left(\pi\frac{r}{\epsilon}\right)^{\frac{1}{2}}} \;\left\| \hat{\Psi}^N \right\|,$$

where

$$\begin{aligned} G_0(\epsilon) \;&:=\; \|f''\|_\infty \left(1 + \left\|h_{\perp,0}^{-1}\right\|_e^2\right)^{1/2} \;+\; 8\,\|f'\|_\infty\, \|\partial_x\, A\|\; \left\|h_{\perp,0}^{-1}\right\|_e \\ &\quad + \; 8\,\|f'\|_\infty \left(\|\partial_x\, A\|^2 \;+\; \epsilon^2 \sup_{y\in[-s,s]} \|\Phi'(y)\|^2 \right)^{1/2}. \end{aligned}$$

The proof of Proposition 1 is based on norm estimates for operators that are rank one in $\mathcal{H}_e$ for each x. In particular, let $\mathcal{R} : \mathbb{R} \to \mathcal{H}_e$ be continuous (or just locally $L^2(\mathbb{R}, \mathcal{H}_e)$). Then clearly $f(x)\mathcal{R}(x) \in L^2(\mathbb{R}, \mathcal{H}_e)$, where f is a cut–off function. Furthermore, $f(x)\,\langle \mathcal{R}(x),\;\cdot\,\rangle : L^2(\mathbb{R}, \mathcal{H}_e) \to L^2(\mathbb{R})$ is a bounded linear operator. Since

$$\begin{aligned} \|f(x)\,\langle \mathcal{R}(x),\, \Psi(x)\rangle\|^2 \;&=\; \int_{\mathbb{R}} f^2(x)\;\; |\langle \mathcal{R}(x),\, \Psi(x)\rangle|^2\; dx \\ &\leq\; \int_{\mathbb{R}} f^2(x)\;\; \|\mathcal{R}(x)\|_e^2\;\; \|\Psi(x)\|_e^2\; dx \\ &\leq\; \sup_{y\in \mathrm{supp}\,(f)} \|\mathcal{R}(y)\|_e^2 \int_{\mathbb{R}} \|\Psi(x)\|_e^2\; dx., \end{aligned}$$

we have,

$$\|f(x)\,\langle \mathcal{R}(x),\;\cdot\,\rangle\| \;\leq\; \sup_{y\in \mathrm{supp}\,(f)} \|\mathcal{R}(y)\|_e.$$

Further consequences of this result are summarized in the following lemma:

Lemma 4 *Let $\mathcal{R}$ be an analytic $\mathcal{H}_e$–valued function, defined on the region S'' (which depends on $s > 0$, $1 \geq \delta > 0$ and $\mu > 0$). Let f be a cut–off function with support on $[-s/\epsilon, s/\epsilon]$. Then there exists a constant $M_{\mathcal{R}} > 0$, independent of $\epsilon > 0$, such that:*

(i) $\|\, f(x)\; \langle \mathcal{R}(\epsilon x),\;\cdot\,\rangle \,\| \;\leq\; M_{\mathcal{R}}$.

(ii) For each $\eta \in (-|x|, |x|)$ and any pair of integers j and l that satisfy $j \leq i$ and $j + l \leq 0$,

$$\left\| f(x)\,\frac{x^{j+l}}{j!}\; \left\langle \mathcal{R}^{(j)}(\epsilon\eta),\, U(P_{i\leq n}\otimes I)U^\star\;\cdot\, \right\rangle \right\| \;\leq\; M_{\mathcal{R}}\;\delta^{-j}\; 2^{\frac{j+l}{2}} \left[\frac{(n+j+l)!}{n!}\right]^{1/2}.$$

Proof: Statement (i) is obvious. To prove (ii), first note that

$$\left\| f(x)\,\frac{x^{j+l}}{j!}\,\left\langle \mathcal{R}^{(j)}(\epsilon\eta),\, U(P_{i\le n}\otimes I)U^\star\,\cdot\,\right\rangle \right\| \;\le\; \left\| f(x)\,\frac{1}{j!}\,\left\langle \mathcal{R}^{(j)}(\epsilon\eta),\;\cdot\,\right\rangle \right\|\;\left\| x^{j+l}P_{i\le n}\right\|.$$

Now use (i), the Cauchy Integral Formula to estimate $\left\|\mathcal{R}^{(j)}(\epsilon\eta)\right\|_e/j!$, and Lemma 5.1 of [7] to estimate $\left\|x^{j+l}P_{i\le n}\right\|$. ☐

A similar result holds for analytic complex–valued functions, which we state without proof.

Lemma 5 *Let $\mathcal{D}$ be an analytic complex–valued function, defined on the region S''. Under the same conditions as stated in Lemma 4, there exists a constant $M_{\mathcal{D}}>0$, independent of $\epsilon>0$, such that:*

(i) $\|\, f(x)\,\mathcal{D}(\epsilon x)\,\| \;\le\; M_{\mathcal{D}}$.

(ii) For each $\eta\in(-|x|,\,|x|)$ and any pair of integers j and l that satisfy $j\le i$ and $j+l\le 0$,

$$\left\| f(x)\;\frac{x^{j+l}}{j!}\;\mathcal{D}^{(j)}(\epsilon\eta)\;P_{i\le n}\right\| \;\le\; M_{\mathcal{D}}\;\delta^{-j}\;2^{\frac{j+l}{2}}\;\left[\frac{(n+j+l)!}{n!}\right]^{1/2}.$$

Sketch of the proof of Proposition 1: We have

$$\begin{aligned}
\|f\,S_N\| \;\le\; & \sum_{m=0}^{N}\epsilon^{m+3}\;\left\|\, f\,\left\langle \mathcal{A}^{[N-m-1]},\,\partial_x\Psi_{\perp,m}\right\rangle\right\| \\
&+\epsilon^{N+4}\;\left\|\, f\,\left\langle \mathcal{A}^{[-1]},\,\partial_x\Psi_{\perp,N+1}\right\rangle\right\| \;+\;\epsilon^{N+5}\;\left\|\, f\,\left\langle \mathcal{A}^{[-1]},\,\partial_x\Psi_{\perp,N+2}\right\rangle\right\| \\
&+\frac{1}{2}\sum_{m=0}^{N-1}\epsilon^{m+4}\;\left\|\, f\,\mathcal{B}^{[N-m-2]}\,w_m\right\| \;+\;\frac{\epsilon^{N+4}}{2}\;\left\|\, f\,\mathcal{B}^{[-1]}\,w_N\right\| \\
&+\frac{1}{2}\sum_{m=0}^{N-1}\epsilon^{m+4}\;\left\|\, f\left\langle \mathcal{C}^{[N-m-2]},\,\Psi_{\perp,m}\right\rangle\right\| + \frac{\epsilon^{N+4}}{2}\;\left\|\, f\left\langle \mathcal{C}^{[-1]},\,\Psi_{\perp,N}\right\rangle\right\| \\
&+\frac{\epsilon^{N+5}}{2}\;\left\|\, f\left\langle \mathcal{C}^{[-1]},\,\Psi_{\perp,N+1}\right\rangle\right\| \;+\;\frac{\epsilon^{N+6}}{2}\;\left\|\, f\left\langle \mathcal{C}^{[-1]},\,\Psi_{\perp,N+2}\right\rangle\right\| \\
&+\sum_{m=0}^{N}\epsilon^{m}\;\left\|\, f\,\mathcal{E}^{[N-m+2]}\,w_m\right\| \;+\;\sum_{l=N+3}^{2N+2}\epsilon^{l}\;\sum_{m=l-N-2}^{N}\;|E_{l-m}|\;\|w_m\|\,. \qquad (10)
\end{aligned}$$

We now apply Lemma 4, Lemma 5, and Theorem 2. This leads to an upper bound for $\|f\,S_N\|$ that looks nearly identical to the right-hand side of inequality (30) of [9]. The statement of the proposition then follows from the proof of Theorem 3 of that paper. ☐

Sketch of the proof of Proposition 2: The strategy is the same as for Proposition 1. However, there is a complication because our expression for T_N contains more terms than in the corresponding expression in [9].

By the triangle inequality and our expression for T_N, we have

$$\begin{aligned}
\|f\,T_N\| \;=\;& \frac{1}{2}\,\epsilon^{N+3}\;\left\|\,f\;\partial_x^2\,\Psi_{\perp,N+1}\,\right\| \;+\; \frac{1}{2}\,\epsilon^{N+4}\;\left\|\,f\;\partial_x^2\,\Psi_{\perp,N+2}\,\right\| \\
&+\sum_{m=0}^{N}\,\epsilon^{m+3}\;\left\|\,f\;(\partial_x\,w_m)\,\mathcal{A}^{[N-m-1]}\,\right\| \;+\; \sum_{m=0}^{N}\,\epsilon^{m+3}\;\left\|\,f\;\mathcal{G}^{[N-m-1]}\;\partial_x\,\Psi_{\perp,m}\,\right\| \\
&+\epsilon^{N+4}\;\left\|\,f\;\mathcal{G}^{[-1]}\;\partial_x\,\Psi_{\perp,N+1}\,\right\| \;+\; \epsilon^{N+5}\;\left\|\,f\;\mathcal{G}^{[-1]}\;\partial_x\,\Psi_{\perp,N+2}\,\right\| \\
&+\frac{1}{2}\sum_{m=0}^{N-1}\,\epsilon^{m+4}\;\left\|\,f\;\mathcal{F}^{[N-m-2]}\;w_m\,\right\| \;+\; \frac{\epsilon^{N+4}}{2}\;\left\|\,f\;\mathcal{F}^{[-1]}\;w_N\,\right\| \\
&+\frac{1}{2}\sum_{m=0}^{N-1}\,\epsilon^{m+4}\;\left\|\,f\;\mathcal{K}^{[N-m-2]}\;\Psi_{\perp,m}\,\right\| \;+\; \frac{\epsilon^{N+4}}{2}\;\left\|\,f\;\mathcal{K}^{[-1]}\;\Psi_{\perp,N}\,\right\| \\
&+\frac{\epsilon^{N+5}}{2}\;\left\|\,f\;\mathcal{K}^{[-1]}\;\Psi_{\perp,N+1}\,\right\| \;+\; \frac{\epsilon^{N+6}}{2}\;\left\|\,f\;\mathcal{K}^{[-1]}\;\Psi_{\perp,N+2}\,\right\| \\
&+\sum_{m=0}^{N+2}\,\epsilon^{m}\;\left\|\,f\;h_{\perp}^{[N-m+2]}\;\Psi_{\perp,m}\,\right\| \;+\; \sum_{l=N+3}^{2N+4}\,\epsilon^{l}\sum_{m=l-N-2}^{N+2}\,|E_{l-m}|\;\|\Psi_{\perp,m}\|\,. \qquad (11)
\end{aligned}$$

We refer to the terms in this expression (in order) as terms 1, 2, ..., 14. Terms 1–3, 7–14 are completely analogous to terms 1–11 of equation (35) of [9] (in the same order), and they respectively satisfy the corresponding bounds as in [9]. As with Proposition 1 the proof of this requires the use of Lemmas 4, 5 (with slight modifications), and Theorem 2. Terms 4–6 in (11) do not occur in equation (35) of [9], but they arise in the same way as the first three terms in (10) (or equivalently as the first four terms in equation (35) of [9]). Since the operator norms of $\mathcal{G}^{[j]}$ and vector norms of $\mathcal{A}^{[j]}$ satisfy the same types of bounds, the norms of terms 4–6 of (11) satisfy the same bounds as the norms of the first three terms of (10).

The Proposition follows since the norm of every term in (11) is bounded by some constant times $F_2^m\,\epsilon^m\,[(m+\alpha+1)!]^{1/2}$, for some F_2, where $N+2\le m\le 2N+2$. □

Proposition 3 is essentially a consequence of $\chi_{f'}$ picking up only the exponentially decaying portion of the lower–order eigenfunctions of the harmonic oscillator Hamiltonian H_0. More precisely, we have the following lemma.

Lemma 6 *For any non-negative integer n and every $\epsilon>0$ that satisfy $r^2/\epsilon^2\ge 2n+1$, we have*

$$\|\,\chi_{f'}\;P_{i\le n}\,\|\;<\;\frac{2^n\;\exp\left(-\frac{r^2}{2\epsilon^2}\right)}{\left(\pi\,\frac{r}{\epsilon}\right)^{\frac{1}{2}}}.$$

Proof: Consider any $\varphi = \sum_{i=0}^{n} d_i\, \phi_i$, where the ϕ_i's are the normalized eigenfunctions of H_0. Then,

$$\|\,\chi_{f'}\,P_{i\leq n}\,\varphi\,\| \;\leq\; \sum_{i=0}^{n} |d_i|\;\|\,\chi_{f'}\phi_i\,\| \;\leq\; \left(\sum_{i=0}^{n} |d_i|^2\right)^{\frac{1}{2}} \left(\sum_{i=0}^{n} \|\,\chi_{f'}\,\phi_i\,\|^2\right)^{\frac{1}{2}}.$$

Therefore,

$$\|\,\chi_{f'}\,P_{i\leq n}\,\| \;\leq\; \left(\sum_{i=0}^{n} \|\,\chi_{f'}\,\phi_i\,\|^2\right)^{\frac{1}{2}}.$$

Recall that $\phi_i(x) = \sqrt{\pi^{1/2}\,2^i\,i!}\;\exp(-x^2/2)\;H_i(x)$, where the Hermite polynomials $H_i(x)$ satisfy the inequality $|H_i(x)| \leq 2^i|x|^i$ for $x \geq \sqrt{2i+1}$, as proved in Lemma 3.1 of [6]. Thus,

$$\begin{aligned}
\sum_{i=0}^{n} \|\,\chi_{f'}\,\phi_i\,\|^2 \;&=\; \sum_{i=0}^{n} \int_{\mathbb{R}} \chi_{f'}(x)\;|\phi_i(x)|^2\;dx \\
&\leq\; 2\,\sum_{i=0}^{n} \int_{r/\epsilon}^{\infty} |\phi_i(x)|^2\;dx \\
&\leq\; \frac{2}{\pi^{1/2}}\;\sum_{i=0}^{n} \frac{2^i}{i!} \int_{r/\epsilon}^{\infty} e^{-x^2}\;x^{2i}\;dx \\
&<\; \frac{2}{\pi^{1/2}}\;4^n \int_{r/\epsilon}^{\infty} e^{-x^2} \sum_{i=0}^{n} \frac{1}{i!}\left(\frac{x^2}{2}\right)^{i}\;dx \\
&<\; \frac{2}{\pi^{1/2}}\;4^n \int_{r/\epsilon}^{\infty} e^{-x^2/2}\;dx.
\end{aligned}$$

Finally, use inequality 7.1.13 of [1] to complete the proof. □

Proof of Proposition 3: We have

$$\begin{aligned}
\left\|\!\left|\,[\partial_x^2, f]\;\Psi^N\right\|\!\right| \;&\leq\; \left\|\!\left|f''\,\Psi^N\right\|\!\right| \;+\; 2\;\left\|\!\left|f'\,\partial_x\,\Psi^N\right\|\!\right| \\
&\leq\; \|f''\|_\infty \left\|\!\left|\chi_{f'}\,\Psi^N\right\|\!\right| \;+\; 2\,\|f'\|_\infty \left\|\!\left|\chi_{f'}\,\partial_x\,\Psi^N\right\|\!\right|.
\end{aligned}$$

The first term is estimated as follows:

$$\begin{aligned}
\left\|\!\left|\chi_{f'}\,\Psi^N\right\|\!\right|^2 \;&=\; \left\|\chi_{f'}\,w^N\right\|^2 \;+\; \left\|\!\left|\chi_{f'}\,\Psi^N_\perp\right\|\!\right|^2 \\
&\leq\; \left\|\chi_{f'}\,A\,P_{i\leq 3N+\alpha}\right\|^2 \left\|\hat{w}^N\right\|^2 \;+\; \left\|\!\left|\chi_{f'}\,h_{\perp,0}^{-1}\,U(A\,P_{i\leq 3N+\alpha-2}\otimes I)U^\star\right\|\!\right|^2 \left\|\!\left|\hat{\Psi}^N_\perp\right\|\!\right|^2 \\
&\leq\; \left\|\chi_{f'}\,P_{i\leq 3N+\alpha}\right\|^2 \left\|\hat{w}^N\right\|^2 \;+\; \left\|h_{\perp,0}^{-1}\right\|_e^2 \left\|\chi_{f'}\,P_{i\leq 3N+\alpha-2}\right\|^2 \left\|\!\left|\hat{\Psi}^N_\perp\right\|\!\right|^2 \\
&<\; \left(1 \;+\; \left\|h_{\perp,0}^{-1}\right\|_e^2\right) \left\|\chi_{f'}\,P_{i\leq 3N+\alpha}\right\|^2 \left\|\!\left|\hat{\Psi}^N\right\|\!\right|^2.
\end{aligned}$$

The second term requires a little more work. We have,

$$\left\|\!\left|\chi_{f'}\,\partial_x\,\Psi^N\right|\!\right\| \;\le\; \left\|\!\left|\chi_{f'}\,\partial_x\left(w^N\,\Phi\right)\right|\!\right\| \;+\; \left\|\!\left|\chi_{f'}\,\partial_x\,\Psi_\perp^N\right|\!\right\|.$$

Since $\langle\Phi,\,\Phi'\rangle = 0$, it follows that

$$\left\langle\partial_x\left(w^N\,\Phi\right),\,\partial_x\left(w^N\,\Phi\right)\right\rangle \;=\; \left|\partial_x\,w^N\right|^2 \;+\; \epsilon^2\,\left|w^N\right|^2\|\Phi'\|_e^2.$$

Therefore,

$$\begin{aligned}
\left\|\!\left|\chi_{f'}\,\partial_x\left(w^N\,\Phi\right)\right|\!\right\|^2 \;&=\; \left\|\chi_{f'}\,\partial_x\,w^N\right\|^2 \;+\; \epsilon^2\int_{\mathbb{R}}\chi_{f'}\,\left|w^N\right|^2\|\Phi'\|_e^2\,dx\\
&\le\; \left\|\chi_{f'}\,\partial_x\,w^N\right\|^2 \;+\; \epsilon^2\sup_{x\in[-s/\epsilon,s/\epsilon]}\|\Phi'(\epsilon x)\|_e^2\left\|\chi_{f'}\,w^N\right\|^2\\
&<\; \|\chi_{f'}\,P_{i\le 3N+\alpha+1}\|^2\left(\|\partial_x\,A\|^2 \;+\; \epsilon^2\sup_{y\in[-s,s]}\|\Phi'(y)\|_e^2\right)\left\|\hat{w}^N\right\|^2\\
&\le\; \|\chi_{f'}\,P_{i\le 3N+\alpha+1}\|^2\left(\|\partial_x\,A\|^2 \;+\; \epsilon^2\sup_{y\in[-s,s]}\|\Phi'(y)\|_e^2\right)\left\|\!\left|\hat{\Psi}^N\right|\!\right\|^2.
\end{aligned}$$

On the other hand,

$$\begin{aligned}
\left\|\!\left|\chi_{f'}\,\partial_x\,\Psi_\perp^N\right|\!\right\| \;&=\; \left\|\!\left|\chi_{f'}\,\partial_x\,h_{\perp,0}^{-1}\,\tilde{A}\,\hat{\Psi}_\perp^N\right|\!\right\|\\
&\le\; \left\|h_{\perp,0}^{-1}\right\|_e\left\|\!\left|\chi_{f'}\,\partial_x\,U(A\,P_{i\le 3N+\alpha-2}\otimes I)U^\star\,\hat{\Psi}_\perp^N\right|\!\right\|\\
&\le\; \left\|h_{\perp,0}^{-1}\right\|_e\|\chi_{f'}\,\partial_x\,A\,P_{i\le 3N+\alpha-2}\|\left\|\!\left|\hat{\Psi}_\perp^N\right|\!\right\|\\
&\le\; \left\|h_{\perp,0}^{-1}\right\|_e\|\chi_{f'}\,P_{i\le 3N+\alpha-1}\|\,\|\partial_x\,A\|\left\|\!\left|\hat{\Psi}^N\right|\!\right\|.
\end{aligned}$$

We now put all the pieces together and use Lemma 6. □

An immediate consequence of Propositions 1–3 is:

Theorem 3 *There exist constants G, F, and Q such that*

$$\left\|\!\left|\left(H(\epsilon)-E^N\right)\Xi^N\right|\!\right\| \;<\; \sum_{m=N+3}^{2N+4} G\,F^m\,\epsilon^m\,[(m+\alpha+1)!]^{1/2} \;+\; Q\,2^{3N}\,\exp\left(-\frac{r^2}{2\epsilon^2}\right)\left\|\!\left|\hat{\Psi}^N\right|\!\right\|, \quad (12)$$

for every $N\ge 3$ and $1\ge\epsilon>0$ that satisfy the inequality $r^2/\epsilon^2\ge 6N+2\alpha+3$.

An easy estimate for $\left\|\hat{\Psi}^N\right\|$, which follows from Theorem 2, together with a redefinition of the constants G and F, yield the following inequality:

$$\left\| \left(H(\epsilon) - E^N\right) \Xi^N \right\| < \exp\left(-\frac{r^2}{2\epsilon^2}\right) \sum_{m=0}^{N+2} GF^m \epsilon^m \left[(m+\alpha+1)!\right]^{1/2} + \sum_{m=N+3}^{2N+4} GF^m \epsilon^m \left[(m+\alpha+1)!\right]^{1/2},$$

also valid under the conditions given in Theorem 3. This inequality is the starting point for the proof of our main result:

Theorem 4 *Let r and F be the constants defined above. Assume $\epsilon_0 > 0$ is small enough to satisfy the inequality $r^2/\epsilon_0^2 \geq 6N + 2\alpha + 3$ with $N \geq 3$. Define $X = \min\{F^{-2}, r^2/3\}$. Then, for every g that satisfies $0 < g < X$ and for every $\epsilon_0 \geq \epsilon > 0$, there exists $N(\epsilon)$ that behaves like g/ϵ^2, such that*

$$\left\| \left(H(\epsilon) - E^{N(\epsilon)}\right) \Xi^{N(\epsilon)} \right\| \ < \ \Lambda \exp\left(-\Gamma/\epsilon^2\right).$$

for some $\Lambda > 0$ and $\Gamma > 0$ independent of ϵ.

Proof: Choose $0 < g < X$. Then $gF^2 = e^{-\zeta}$ for some $\zeta > 0$. Set $N(\epsilon) = [\![g/2\epsilon^2 - \alpha/2 - 5/2]\!]$. Then $N(\epsilon)$ satisfies both $r^2/\epsilon^2 \geq 6N(\epsilon) + 2\alpha + 3$ and $g/\epsilon^2 - \alpha - 5 \geq 2N(\epsilon) \geq g/\epsilon^2 - \alpha - 7$.

Stirling's formula implies

$$\sum_{m=M_1}^{M_2} G\, F^m\, \epsilon^m \left[(m+\alpha+1)!\right]^{1/2} \ < \ \Lambda_0 \sum_{m=M_1}^{M_2} m^{1/4}\, e^{-m} \left[F^2\, \epsilon^2\, (m+\alpha+1)\right]^{(m+\alpha+1)/2},$$

where Λ_0 is some appropiate constant, and the sum range $[M_1,\, M_2]$ is either $[1,\, N(\epsilon)+2]$ or $[N(\epsilon)+3,\, 2N(\epsilon)+4]$ (the term with $m = 0$ is ignored without consequence). Now, since $m \leq 2N(\epsilon) + 4 \leq g/\epsilon^2 - \alpha - 1$,

$$\begin{aligned}
\sum_{m=M_1}^{M_2} m^{1/4} e^{-m} \left[F^2\, \epsilon^2\, (m+\alpha+1)\right]^{(m+\alpha+1)/2} \ &\leq \ \sum_{m=M_1}^{M_2} m^{1/4} e^{-m} (gF^2)^{(m+\alpha+1)/2} \\
&= \ \sum_{m=M_1}^{M_2} m^{1/4} e^{-m} e^{-\zeta(m+\alpha+1)/2} \\
&< \ e^{-\zeta(M_1+\alpha+1)/2} \sum_{m=1}^{\infty} m^{1/4} e^{-m},
\end{aligned}$$

where the series in the last inequality is clearly convergent. It thus follows that

$$\left\| \left(H(\epsilon) - E^{N(\epsilon)}\right) \Xi^{N(\epsilon)} \right\| \ < \ \Lambda_1 \exp\left(-\frac{r^2}{2\epsilon^2}\right) + \Lambda_2 \exp\left(-\frac{\zeta g}{2\epsilon^2}\right),$$

for some Λ_1 and Λ_2. □

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