Exponentially Accurate Error Estimates of Quasiclassical Eigenvalues II: Several Dimensions

J H Toloza* †

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Abstract

We study the behavior of truncated Rayleigh-Schrödinger series for low-lying eigenvalues of the time-independent Schrödinger equation, in the semiclassical limit $\hbar \searrow 0$. In particular we prove that if the potential energy satisfies certain conditions, there is an optimal truncation of the series for the eigenvalues, in the sense that this truncation is exponentially close to the exact eigenvalue. These results were already discussed for one-dimensional case in a previous paper. This time we consider the several dimensional case, where degeneracy plays a central role.

1 Introduction

The semiclassical aproximation has been extensively exploited in the study of the time independent Schrödinger equation [5]

$$\left[-\frac{\hbar^2}{2}\Delta_x + V(x)\right]\tilde{\Psi}(x) = E\tilde{\Psi}(x) \tag{1}$$

In particular, existence of low-lying eigenvalues was proved for potential wells in the limit of small $\hbar > 0$ [1, 6, 13]. It is also shown that the eigenvalues and eigenvectors admit asymptotics expansions to all orders, given by formal Rayleigh-Schrödinger (R-S) series. The papers [1, 6] deal with the one-dimensional problem, the former by resorting to the Krein's formula and the latter by applying the "twisting trick" [11, 2]. The several dimensional case is discussed in [13], by means of geometric arguments.

In all cases, the potential energy $V(x)$ is supposed to admit a second order approximation at each global miminum. Those terms are separated from the potential energy term, and a suitable scaling is made on the Schrödinger equation. The quadratic pieces along with the

*Department of Physics and Center for Statistical Mechanics and Mathematical Physics, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061-0435, USA

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kinetic energy term are treated as an "unperturbed" harmonic oscillator halmitonian, and the remainder is considered as a perturbation of it. Then the mathematical machinery developed in [9] (also in [12]) is used.

However, no results were known about the behavior of truncations of these series, which one expects to be good aproximations to the solutions of (1). In [15] we have discussed this issue for the one-dimensional problem. In this paper we extend those results to the several dimensional case. To that end, we consider the time independent Schrödinger equation (1) in d dimensions where $x = (x_1, \ldots, x_d)$, in the semiclassical limit $\hbar \searrow 0$. We assume that the potential $V(x)$ satisfies the following conditions:

H1. Let $V(x)$ be a C^∞ real function on $\mathbb{R}^d$, with a unique global minimum $V(0) = 0$ at $x = 0$, and $\liminf_{|x|\to\infty} V(x) > 0$. The global minimum is non-degenerate in the sense that the matrix

$$A_{ij} := \frac{\partial^2 V}{\partial x_i \partial x_j}(0)$$

has only strictly positive eigenvalues $\omega_1, \ldots, \omega_d$. Let us denote the lowest eigenvalue as ω_0.

H2. $V(x)$ has an analytic extension to a neighborhood of the region $S_\delta = \{z : |\mathrm{Im}\, z_i| \leq \delta\}$ and satisfies $|V(z)| \leq M \exp(\tau |z|^2)$ when $z \in S_\delta$, for some positive constants M and $\tau \leq \omega_0/4$.

Our goal is to prove that for sufficiently small values of $\hbar$ there is an optimal truncation of the perturbation series, in the sense that the difference between an approximate and actual eigenvalue is smaller than $\exp(-\text{constant}/\hbar)$ for some positive constant. In this paper we follow the method explained in [15]. This indeed is related with one developed in [3] to study approximate solutions to the time dependent Schrödinger equation – a problem related to the one investigated here. Roughly speaking, we calculate upper bounds for each term in the R-S series for both eigenvalues and eigenfuctions. Then we combine these to obtain a recursion relation that yields an estimate for the growth of these terms. From that we compute an estimate of the difference of the two sides of (1) after truncation at order N; this estimate behaves like $ab^N \hbar^{\frac{N}{2}} (N!)^{\frac{1}{2}}$. For each $\hbar$ we choose N to minimize this quantity. This and some standard results of functional analysis yield our results. The main change with respect to [15] comes from the fact that, in several dimensions, we need to consider degenerate perturbation theory. There are also several technical nuissances which require special treatment.

Hypothesis H1 ensures existence of discrete spectrum near of the bottom of $V(x)$, for sufficiently small $\hbar > 0$ [13]. The uniqueness of the global minimum is required essentially to avoid dealing with "cut-off at large distance" which would make our results more difficult to present. Indeed, in [1, 13] the potential $V(x)$ is allowed to have multiple wells, which yields tunneling (see e. g., [1, 14, 4] and references therein).

Hypothesis H2 allows us to control the growth of derivatives of $V(x)$ far from the potential well. That is needed in order to obtain an upper bound to the error committed by inserting truncated series into equation (1), since it involves evaluation of integrals of the form

$$\int_{\mathbb{R}^d} \text{Polynomial}(x)\, |D^m V(x)|\, e^{-c|x|^2} d^d x.$$

This paper is organized as follows. In Section 2 we make a transformation of equation (1), and some technical results are proven. In Section 3 we construct some operators through recursion relations, which allow us to calculate the several correction terms involved in the formal series for eigenvalues and eigenvectors. In particular, this construction allows us to consider the cases where degeneracy occurs. Because of the tranformation done in Section 2, we obtain a manageable recursion relation for the n^{th} term of the R-S series. Then we state and prove an estimate of the growth of these terms. In section 4 we define a residual error function for equation (1) and prove an estimate for it. The main results are stated precisely in Section 5. The Appendix is devoted to a computation needed in Section 4.

2 Preliminaries

We first transform (1) by scaling $x \to \hbar^{\frac{1}{2}} x$ and then dividing the whole equation by $\hbar$. The transformed equation is

$$\left[-\frac{1}{2}\Delta_x + V(\hbar;x)\right]\tilde{\Psi}(\hbar;x) = E(\hbar)\tilde{\Psi}(\hbar;x) \tag{2}$$

Because of H1, $V(x)$ admits a Taylor expansion up to any order n. Thus we can write

$$V(\hbar;x) = \frac{1}{2}\sum_{i,j=1}^{d} A_{ij}x_i x_j + W(\hbar;x)$$

where the function $W(\hbar;x)$ can be asymptotically approximated by

$$W(\hbar;x) = \sum_{l=3}^{n} \hbar^{\frac{l-2}{2}} \sum_{|m|=l} \frac{D^m V(0)}{m!} x^m + O\left(\hbar^{\frac{n-1}{2}} x^{|m|=n+1}\right), \tag{3}$$

where we use the standard multi-index notation: $m = (m_1, \ldots, m_d)$, $|m| = m_1 + \ldots + m_d$, $x^m = x_1^{m_1} \cdot \ldots \cdot x_d^{m_d}$, $m! = m_1! \cdot \ldots \cdot m_d!$ and $D^m V = \partial_{x_1}^{m_1} \cdot \ldots \cdot \partial_{x_d}^{m_d} V$. Furthermore, H2 implies that the Taylor series (3) is indeed convergent inside an open poly-disc $\{z \in \mathbb{C}^d : |z_i| \le \delta\}$. As a consequence, there is constant $c < \infty$ so that for each multi-index m

$$\frac{|D^m V(0)|}{m!}\delta^{|m|} \le c$$

Then

$$\sum_{|m|=l} \frac{|D^m V(0)|}{m!}\delta^{|m|} \le c \sum_{|m|=l} 1$$

for all l. The last summation is the number of different ways to sum d non-negative integers such as the result is equal to l. That is,

$$\sum_{|m|=l} 1 = \frac{(l+d-1)!}{l!(d-1)!} \le \frac{1}{(d-1)!}(l+d-1)^{d-1}$$

Therefore, we have

$$\sum_{|m|=l} \frac{|D^m V(0)|}{m!} \delta^{|m|} \leq C Y^l$$

for some constants C and Y, which depend only on the dimensional constant d. Without loss we assume that $\delta \leq 1$.

Now we can rewrite (2) as

$$[H_0 + W(\hbar; x)]\, \tilde{\Psi}(\hbar; x) = E(\hbar) \tilde{\Psi}(\hbar; x) \tag{4}$$

where

$$H_0 = -\frac{1}{2}\Delta_x + \frac{1}{2}\sum_{i,j} A_{ij} x_i x_j$$

is a harmonic oscillator hamiltonian with eigenfrequencies $\omega_1, \ldots, \omega_d$. In suitable cartesian coordinates, the eigenfunctions of H_0 can be written as

$$\Phi_j(x) = \pi^{-\frac{1}{4}} \left(2^{|j|} j!\right)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}\sum_{i=1}^{d} \omega_i x_i^2\right) \prod_{i=1}^{d} H_{j_i}\left(\sqrt{\omega_i} x_i\right) \tag{5}$$

where $j = (j_1, \ldots, j_d)$ and $H_{j_i}(y)$ are the Hermite polynomials. The corresponding eigenvalues are $e_j = \sum_{i=1}^{d} \omega_i j_i + d/2$.

In the semiclassical limit we may consider $W(\hbar, x)$ as a perturbation of H_0. Then we can propose formal Rayleigh-Schrödinger series for both $E(\hbar)$ and $\tilde{\Psi}(\hbar; x)$

$$\tilde{\Psi}(x) \sim \tilde{\psi}_0(x) + \hbar^{\frac{1}{2}} \tilde{\psi}_1(x) + \hbar^{\frac{2}{2}} \tilde{\psi}_2(x) + \hbar^{\frac{3}{2}} \tilde{\psi}_3(x) + \hbar^{\frac{4}{2}} \tilde{\psi}_4(x) + \ldots \tag{6}$$

$$E(\hbar) \sim e + \hbar^{\frac{1}{2}} \mathcal{E}_1 + \hbar^{\frac{2}{2}} \mathcal{E}_2 + \hbar^{\frac{3}{2}} \mathcal{E}_3 + \hbar^{\frac{4}{2}} \mathcal{E}_4 + \ldots, \tag{7}$$

where e is an eigenvalue of H_0 with multiplicity g and associated eigenspace B. Later we will find that $\tilde{\psi}_0(x)$ must be a vector in B, as expected.

Before going into the standard physicist-like perturbation procedure, let us make a further transformation of (4). Let $\{\Phi_j(x)\}$ be a basis of eigenvectors of H_0. For a given eigenvalue e of H_0 define a new operator A_e by

$$A_e \Phi_j(x) = \begin{cases} \Phi_j(x) & \text{if } \Phi_j(x) \in B \\ |e - e_j|^{-\frac{1}{2}} \Phi_j(x) & \text{otherwise.} \end{cases}$$

where e_j is the eigenvalue associated with $\Phi_j(x)$. Then extend A_e to the whole Hilbert space $\mathcal{H}$ by linearity. So defined, A_e is a bounded operator with unbounded inverse. Now define $H_e = A_e(H_0 - e)A_e$. This operator satisfies

$$H_e \Phi_j(x) = \begin{cases} 0 & \text{if } \Phi_j(x) \in B \\ \frac{e - e_j}{|e - e_j|} \Phi_j(x) & \text{otherwise.} \end{cases}$$

on an eigenbasis of H_0. With these definitions, (4) transforms into

$$[H_e + A_e W(\hbar; x) A_e] \, \Psi(x) = [E(\hbar) - e] \, A_e^2 \Psi(x) \tag{8}$$

and instead of (6) we have

$$\Psi(x) \sim \psi_0(x) + \hbar^{\frac{1}{2}} \psi_1(x) + \hbar^{\frac{2}{2}} \psi_2(x) + \hbar^{\frac{3}{2}} \psi_3(x) + \hbar^{\frac{4}{2}} \psi_4(x) + \dots \tag{9}$$

It is easy to prove that each $\tilde{\psi}_n$ lies in a finite-dimensional subspace that is in the domain of A_e^{-1}. Thus each term of (9) is related to those in (6) through the identity $\tilde{\psi}_n = A_e \psi_n$. We make this transformation because it yields better estimates to the growth of the R-S coefficients. Furthermore, we need only to transform back the solution for the eigenvector via the operator A_e.

Now insert (9) and (7) into (8) and equate powers of $\hbar^{\frac{1}{2}}$. The zeroth-order equation yields $H_e \psi_0 = 0$ so $\psi_0 \in B$. For $n = 1, 2, \dots$, we have

$$H_e \psi_n + \sum_{l=1}^{n} T^{(l+2)} \psi_{n-l} = \sum_{l=1}^{n} \mathcal{E}_l A_e^2 \psi_{n-l} \tag{10}$$

where

$$T^{(l)} := \sum_{|m|=l} \frac{1}{m!} D^m V(0) A_e x^m A_e \tag{11}$$

Depending on what the eigenfrequencies of H_0 actually are, we might need to deal with degenerate perturbation theory. Furthermore in that case, the degeneracy may be partly or totally preserved by the perturbation term $W(\hbar, x)$, as happens when $W(\hbar, x)$ has some of the symmetries of H_0. Because of the multiple possibilities, the computation of the several correction terms for both (9) and (7) is rather involved; the next section is devoted to it.

Before concluding this section, let us state some technical results. First, define $a = a_e$ to be the smallest non-negative integer such that $B \subseteq \mathrm{Ran}\left(P_{|j| \le a}\right)$, where $P_{|j| \le l}$ is the projection onto the subspace spanned by $\{ \Phi_j \, : \, |j| \le l \}$.

Lemma 1 *For $n \ge 1$, ψ_n exists and $\psi_n \in \mathrm{Ran}\left(P_{|j| \le a+3n}\right)$*

Proof. First, decompose $\psi_n = P_{|j| \le a} \psi_n + \left(1 - P_{|j| \le a}\right) \psi_n =: \psi_n^{(1)} + \psi_n^{(2)}$. We have to prove the statement only for $\psi_n^{(2)}$. Equation (10) yields

$$\psi_n^{(2)} = (H_e)_r^{-1} \left(1 - P_{|j| \le a}\right) \left[\sum_{l=1}^{n} \mathcal{E}_l A_e^2 \psi_{n-l} - \sum_{l=1}^{n} T_e^{(l+2)} \psi_{n-l} \right]$$

where $(H_e)_r^{-1}$ is the inverse of the restriction of H_e to $\mathrm{Ran}\left(1 - P_{|j| \le a}\right)$. Since

$$\mathrm{Ran}\left((H_e)_r^{-1} \left(1 - P_{|j| \le a}\right) P_{|j| \le a+3n} \right) \subset \mathrm{Ran}\left(P_{|j| \le a+3n}\right),$$

it is sufficient to show that

$$\left(\sum_{l=1}^{n}\mathcal{E}_l A_e^2\psi_{n-l}-\sum_{l=1}^{n}T_e^{(l+2)}\psi_{n-l}\right)\in P_{|j|\le a+3n}$$

Now use induction. The first term above is trivial. For the second one, let us note that $\mathrm{Ran}\left(A_eP_{|j|\le a+3n}\right)=\mathrm{Ran}\left(P_{|j|\le a+3n}\right)$. Also, a simple calculation with ladder operators shows that $x^m\varphi\in\mathrm{Ran}\left(P_{|j|\le a+3(n-l)+|m|}\right)$ whenever $\varphi\in\mathrm{Ran}\left(P_{|j|\le a+3(n-l)}\right)$. Finally, we have $3(n-l)+2+l=3n+2(1-l)\le 3n$ for $l=1,\dots,n$. □

Lemma 2 *For $|m|\ge 2$, $n\ge 0$ and some constant $\gamma_1>0$,*

$$\left\|A_ex^mA_eP_{|j|\le n}\right\|\le\gamma_1^2 2^{\frac{|m|-2}{2}}\left[\frac{(n+|m|-1)!}{(n+1)!}\right]^{\frac{1}{2}}$$

As a consequence,

$$\left\|T^{(l)}P_{|j|\le n}\right\|\le\gamma\kappa^{\frac{l-2}{2}}\left[\frac{(n+l-1)!}{(n+1)!}\right]^{\frac{1}{2}}$$

for some $\gamma>0$ and $\kappa\ge 2$.

Proof. For a single coordinate x_α, we have

$$x_\alpha=\frac{1}{\sqrt{2\omega_\alpha}}\left(a_\alpha+a_\alpha^*\right)$$

where a_α and a_α^* are the associated ladder operators.

Consider any $\varphi=\sum_j d_j\Phi_j$, $\sum_j|d_j|^2<\infty$. Define $J_B:=\{\text{multi-indices}\, j:\Phi_j\in B\}$. Then

$$\begin{aligned}a_\alpha^*A_e\varphi &= \sum_{j\in J_B}d_ja_\alpha^*\Phi_j+\sum_{j\notin J_B}d_j|e-e_j|^{-\frac{1}{2}}a_\alpha^*\Phi_j\\ &= \sum_{j\in J_B}d_j\sqrt{j_\alpha+1}\Phi_{j+1\alpha}+\sum_{j\notin J_B}d_j|e-e_j|^{-\frac{1}{2}}\sqrt{j_\alpha+1}\Phi_{j+1\alpha}\end{aligned}$$

where $j+1\alpha=(j_1,\dots,j_\alpha+1,\dots,j_d)$. Thus,

$$\begin{aligned}\|a_\alpha^*A_e\varphi\|^2 &= \sum_{j\in J_B}|d_j|^2(j_\alpha+1)+\sum_{j\notin J_B}|d_j|^2|e-e_j|^{-1}(j_\alpha+1)\\ &\le (1+a)\sum_{j\in J_B}|d_j|^2+\sum_{j\notin J_B}|d_j|^2|e-e_j|^{-1}(j_\alpha+1)\end{aligned}$$

because $j\in J_B\Rightarrow j_\alpha\le|j|\le a$. Also,

$$\frac{j_\alpha+1}{|e-e_j|}=\frac{1}{\omega_\alpha}\frac{\omega_\alpha(j_\alpha+1/2)}{|e-e_j|}+\frac{1/2}{|e-e_j|}\le\frac{1}{\omega_\alpha}\frac{e_j}{|e-e_j|}+\frac{1/2}{|e-e_j|}$$

Since $\sigma(H_0)$ has no accumulation points and $e_j \neq e$ for all $j \notin J_B$, $\inf_{j\notin J_B} |e-e_j| > 0$. Since furthermore $\lim_{|j|\to\infty} e_j|e-e_j|^{-1} = 1$, $\sup_{j\notin J_B} e_j|e-e_j|^{-1} < \infty$. Thus,

$$|e-e_j|^{-1}(j_\alpha+1) \leq \frac{1}{\omega_\alpha} \sup_{j\notin J_B} e_j|e-e_j|^{-1} + \frac{1}{2} \sup_{j\notin J_B} |e-e_j|^{-1} =: K_1 < \infty$$

which implies

$$\|a_\alpha^* A_e\|^2 \leq \max\{(1+a), K_1\} \leq \max_{\{\omega_i\}} \max\{(1+a), K_1\} \tag{12}$$

A similar calculation yields,

$$\|a_\alpha A_e\|^2 \leq \max\{|1-a|, K_2\} \leq \max_{\{\omega_i\}} \max\{|1-a|, K_2\} \tag{13}$$

for some $K_2 < \infty$. Therefore,

$$\|x_\alpha A_e\| \leq \frac{1}{\sqrt{2\omega_a}} \|a_\alpha A_e\| + \frac{1}{\sqrt{2\omega_a}} \|a_\alpha A_e^*\| \leq \gamma_1$$

where γ_1 is the sum of the right-hand sides of (12) and (13). Taking the adjoint yields

$$\|A_e x_\alpha\| \leq \gamma_1$$

Since $|m| \geq 2$, we can write $x^m = x_\alpha x^{m'} x_\beta$ for some x_α, x_β, with $|m'| = |m| - 2$. Then

$$\begin{aligned}
\left\|A_e x^m A_e P_{|j|\leq n}\right\| &\leq \left\|A_e x_\alpha x^{m'} P_{|j|\leq n+1} x_\beta A_e P_{|j|\leq n}\right\| \\
&\leq \|A_e x_\alpha\| \, \|x_\beta A_e\| \left\|x^{m'} P_{|j|\leq n+1}\right\| \\
&\leq \gamma_1^2 2^{\frac{|m'|}{2}} \left[\frac{(n+|m'|+1)!}{(n+1)!}\right]^{\frac{1}{2}} \\
&\leq \gamma_1^2 2^{\frac{|m|-2}{2}} \left[\frac{(n+|m|-1)!}{(n+1)!}\right]^{\frac{1}{2}} \qquad (14)
\end{aligned}$$

where we use Lemma 5.1 of [3] to bound $\left\|x^{m'} P_{|j|\leq n+1}\right\|$. The last statement follows from (11) and (14), along with the definitions $\gamma = C\gamma_1^2\delta^{-2}Y^2$ and $\kappa = 2\delta^{-2}Y^2$. □

3 Computation of R-S coefficients

We essentially follow the standard, formal method to compute R-S coefficients (see e. g., [10, Chapter XVI],) although alternatively one could use Kato [9]. However, this last approach seems rather difficult to implement here, in particular when degeneracy occurs. Concerning asymptotics in degenerate perturbation theory, we must mention the approach developed by Hunziker-Pillet [7]. See also [8] for a more specific treatment for Schrödinger eigenvalue problems.

Let us assume that the zeroth-order eigenvalue e is g-fold degenerate, with associated eigenspace B. We allow g to be equal to 1. Let P be the projector onto B and $Q := 1 - P$.

Up to zeroth-order, ψ_0 can be any vector in B, which we may require to be normalized, $\|\psi_0\| = 1$. Two cases may arise from solving (10) at higher order. Either the zeroth-order degeneracy is preserved at all orders, or it is removed to some extent at higher order. Let us start by discussing the former case, which trivially includes the non-degenerate one.

3.1 Degeneracy is preserved.

Fix $\psi_0 \in B$, with $\|\psi_0\| = 1$. The first-order equation is

$$H_e \psi_1 + T^{(3)} \psi_0 = \mathcal{E}_1 A_e^2 \psi_0 \tag{15}$$

Let us multiply by P. Noting that $PH_e = 0$ and $PA_e^2 \psi_0 = \psi_0$, we obtain

$$PT^{(3)} P \psi_0 = \mathcal{E}_1 \psi_0$$

This is the eigenvalue problem for the finite-dimensional, self-adjoint operator $\Lambda^{(1)} := PT^{(3)}P$. Since we assume that the zeroth-order degeneracy is not broken at any order, $\Lambda^{(1)}$ must have only one eigenvalue. Let us call it α_1. Then $\mathcal{E}_1 = \alpha_1$. Now multiply (15) by Q. We obtain

$$H_e Q \psi_1 = -QT^{(3)} \psi_0$$

Let us introduce more notation. For any vector $\psi \in \mathcal{H}$, define $\psi^{||} := P\psi$ and $\psi^{\perp} := Q\psi$. Also, let $(H_e)_{\perp}$ be the restriction of H_e to $\mathrm{Ran}(Q)$. So defined, $(H_e)_{\perp}$ is invertible. Then we have

$$\psi_1^{\perp} = \Xi^{(1,\perp)} \psi_0$$

where $\Xi^{(1,\perp)} := (H_e)_{\perp}^{-1} \left(-QT^{(3)}\right)$. So far $\psi_1^{||}$ remains undefined.

The second-order equation is

$$H_e \psi_2 + T^{(3)} \psi_1 + T^{(4)} \psi_0 = \mathcal{E}_2 A_e^2 \psi_0 + \alpha_1 A_e^2 \psi_1 \tag{16}$$

Multiply (16) by P. After some algebra involving the definitions of $\Lambda^{(1)}$ and $\Xi^{(1,\perp)}$, we obtain

$$\left(PT^{(3)} \Xi^{(1,\perp)} P + PT^{(4)} P\right) \psi_0 = \mathcal{E}_2 \psi_0$$

Then $\mathcal{E}_2$ has to be equal to the unique eigenvalue of $\Lambda^{(2)} := P\left(T^{(3)} \Xi^{(1,\perp)} + T^{(4)}\right) P$. That is, $\mathcal{E}_2 = \alpha_2$. Now multiply (16) by Q to obtain

$$H_e \psi_2^{\perp} + QT^{(3)} \left(\psi_1^{||} + \psi_1^{\perp}\right) + QT^{(4)} \psi_0 = \alpha_1 A_e^2 \psi_1^{\perp}$$

which yields

$$\psi_2^{\perp} = \Xi^{(2,\perp)} \psi_0 + \Xi^{(1,\perp)} \psi_1^{||}$$

where we define

$$\Xi^{(2,\perp)} := (H_e)_\perp^{-1}\left[\left(\alpha_1 A_e^2 - QT^{(3)}\right)\Xi^{(1,\perp)} + QT^{(4)}\right]$$

and no requirement is imposed on either $\psi_2^{||}$ or $\psi_1^{||}$.

The third-order equation is

$$H_e\psi_3 + T^{(3)}\psi_2 + T^{(4)}\psi_1 + T^{(5)}\psi_0 = \mathcal{E}_3 A_e^2\psi_0 + \alpha_2 A_e^2\psi_1 + \alpha_1 A_e^2\psi_2$$

Following the procedure already described, we obtain

$$\Lambda^{(3)}\psi_0 = \mathcal{E}_3\psi_0$$

where

$$\Lambda^{(3)} := P\left(T^{(3)}\Xi^{(2\perp)} + T^{(4)}\Xi^{(1,\perp)} + T^{(5)}\right)P$$

has only one eigenvalue α_3. Thus $\mathcal{E}_3 = \alpha_3$. Also

$$\psi_3^\perp = \Xi^{(3,\perp)}\psi_0 + \Xi^{(2,\perp)}\psi_1^{||} + \Xi^{(1,\perp)}\psi_2^{||}$$

where

$$\Xi^{(3,\perp)} := (H_e)_\perp^{-1}\left[\left(\alpha_1 A_e^2 - QT^{(3)}\right)\Xi^{(2,\perp)} + \left(\alpha_2 A_e^2 - QT^{(4)}\right)\Xi^{(1,\perp)} - QT^{(5)}\right]$$

and nothing is said about $\psi_3^{||}$, $\psi_2^{||}$ or $\psi_1^{||}$.

As one can see, $\mathcal{E}_n$ and $\psi_n^\perp$ can be calculated through recursive definition of certain operators. The form of these operators is now easy to guess:

Proposition 1 *For $n = 1, 2, \ldots$, recursively define*

$$\begin{aligned}
\Xi^{(1,\perp)} &:= -(H_e)_\perp^{-1}QT^{(3)} \\
\Xi^{(n,\perp)} &:= (H_e)_\perp^{-1}\left[\sum_{p=1}^{n-1}\left(\alpha_{n-p}A_e^2 - QT^{(n+2-p)}\right)\Xi^{(p,\perp)} - QT^{(n+2)}\right]
\end{aligned}$$

where α_l is, by assumption, the unique eigenvalue of

$$\Lambda^{(l)} := PT^{(l+2)}P + \sum_{p=1}^{n-1} PT^{(l+2-p)}\Xi^{(p,\perp)}P$$

Then, given $\psi_0 \in B$, $\mathcal{E}_n = \alpha_n$ and

$$\psi_n = \Xi^{(n,\perp)}\psi_0 + \sum_{p=1}^{n-1}\Xi^{(n-p,\perp)}\psi_p^{||} + \psi_n^{||}$$

where $\psi_1^{||}, \ldots, \psi_n^{||}$ are vectors arbitrarily chosen from B.

This construction will be generalized in Proposition 2, from which the proof of Proposition 1 can be easily read out. To rule out arbitrariness, we set $\psi_n^{||} = 0$ for all $n \geq 1$, which is equivalent to absorbing those vectors into ψ_0.

The recursive expressions for the operators $\Lambda^{(n)}$ and $\Xi^{(n,\perp)}$ can be translated into recursive expressions for $\mathcal{E}_n$ and ψ_n. The result is

$$
\begin{aligned}
\mathcal{E}_n &= \sum_{p=0}^{n-1} \left\langle T^{(n+2-p)} P_{|j|\leq a} \psi_0, \psi_p \right\rangle \\
\psi_n &= (H_e)_\perp^{-1} \left[\sum_{p=1}^{n-1} \left(\mathcal{E}_{n-p} A_e^2 - QT^{(n+2-p)} \right) \psi_p - QT^{(n+2)} \psi_0 \right]
\end{aligned}
$$

Furthermore we can obtain the following inequalities, whose derivation is presented after Proposition 2:

$$
\begin{aligned}
\|\mathcal{E}_n\| &\leq \sum_{l=1}^{n} \left\| T^{(l+2)} P_{|j|\leq a} \right\| \|\psi_{n-l}\| \\
\|\psi_n\| &\leq \sum_{l=1}^{n-1} |\mathcal{E}_l| \, \|\psi_{n-l}\| + \sum_{l=1}^{n} \left\| T^{(l+2)} P_{|j|\leq a+3(n-l)} \right\| \|\psi_{n-l}\|
\end{aligned}
$$

By resorting to Lemma 2, we finally obtain

$$
\begin{aligned}
\|\mathcal{E}_n\| &\leq \gamma \sum_{l=1}^{n} \kappa^{\frac{l}{2}} \left[\frac{(1+a+l)!}{(1+a)!} \right]^{\frac{1}{2}} \|\psi_{n-l}\| \\
\|\psi_n\| &\leq \sum_{l=1}^{n-1} |\mathcal{E}_l| \, \|\psi_{n-l}\| + \gamma \sum_{l=1}^{n} \kappa^{\frac{l}{2}} \left[\frac{(1+a+3n-2l)!}{(1+a+3n-3l)!} \right]^{\frac{1}{2}} \|\psi_{n-l}\|
\end{aligned}
$$

These inequalities are essentially identical to (14) and (15) in [15]. As an inmediate consequence, we have

Theorem 1 *For each $a \geq 0$, there is $b > 0$ so that*

$$
\begin{aligned}
\|\mathcal{E}_n\| &\leq \kappa^{3n} b^n [(1+a+n)!]^{\frac{1}{2}} \\
\|\psi_n\| &\leq \kappa^{3n} b^n [(1+a+n)!]^{\frac{1}{2}}
\end{aligned}
$$

for all $n \geq 1$.

This theorem is shown in [15]. Alternatively, one can use the proof of Theorem 2 below to get somewhat tighter bounds.

3.2 Degeneracy is removed.

Let us examine the case where the zeroth-order degeneracy is partially removed only at first order.

First-order: Now the operator $\Lambda^{(1)} = PT^{(3)}P$ has $k \geq 2$ distinct eigenvalues $\alpha_{1,1}, \dots, \alpha_{1,k}$. Let $B_1, \dots, B_k$ be the corresponding eigenspaces, and let $P^{(1)}, \dots, P^{(k)}$ be their orthogonal projections. Set $\mathcal{E}_1 = \alpha_{1,i}$. Then ψ_0 must lie in B_i. As before, $\psi_1^\perp = \Xi^{(1,\perp)}\psi_0$ with $\Xi^{(1,\perp)} := (H_e)_\perp^{-1}\left(-QT^{(3)}\right)$.

Second-order: Because of the choice for $\mathcal{E}_1$ we have

$$H_e\psi_2 + T^{(3)}\psi_1 + T^{(4)}\psi_0 = \mathcal{E}_2 A_e^2\psi_0 + \alpha_{1,i}A_e^2\psi_1 \tag{17}$$

Multiply (17) by $P^{(j)}$

$$P^{(j)}T^{(3)}\psi_1 + P^{(j)}T^{(4)}\psi_0 = \mathcal{E}_2 P^{(j)}\psi_0 + \alpha_{1,i}P^{(j)}\psi_1 \tag{18}$$

Note that for any vector ψ,

$$\begin{aligned} P^{(j)}T^{(3)}\psi^{||} &= \sum_{l=1}^{k} P^{(j)}PT^{(3)}PP^{(l)}\psi^{||} \\ &= \sum_{l=1}^{k} P^{(j)}\Lambda^{(1)}P^{(l)}\psi^{||} \\ &= \sum_{l=1}^{k} \alpha_{1,l}P^{(j)}P^{(l)}\psi^{||} \\ &= \alpha_{1,j}\psi^{(j)} \end{aligned} \tag{19}$$

where $\psi^{||} = P\psi$ as before. Define $\psi^{(j)} = P^{(j)}\psi$. Then $\psi^{||} = \sum_{j=1}^{k}\psi^{(j)}$. With these definitions, (19) yields

$$\begin{aligned} P^{(j)}T^{(3)}\psi_1 &= P^{(j)}T^{(3)}\psi_1^{||} + P^{(j)}T^{(3)}\psi_1^\perp \\ &= \alpha_{1,j}\psi_1^{(j)} + P^{(j)}T^{(3)}\psi_1^\perp \end{aligned} \tag{20}$$

Now insert (20) into (18). For $j = i$ we have

$$P^{(i)}T^{(4)}\psi_0 + P^{(i)}T^{(3)}\psi_1^\perp = \mathcal{E}_2\psi_0$$

Define

$$\Lambda^{(2,i)} := P^{(i)}\left(T^{(4)} + T^{(3)}\Xi^{(1,\perp)}\right)P^{(i)}$$

Then we obtain $\Lambda^{(2,i)}\psi_0 = \mathcal{E}_2\psi_0$. By assumption $\Lambda^{(2,i)}$ has only one eigenvalue $\alpha_{2,i}$. Therefore $\mathcal{E}_2 = \alpha_{2,i}$.

For $j \neq i$ we have

$$P^{(j)}T^{(4)}\psi_0 + P^{(j)}T^{(3)}\psi_1^{\perp} + \alpha_{1,j}\psi_1^{(j)} = \alpha_{1,i}P^{(j)}\psi_1$$

because $P^{(j)}\psi_0 = 0$ whenever $j \neq i$. Rearranging terms we finally obtain $\psi_1^{(j)} = \Xi^{(1,j)}\psi_0$, where we define

$$\Xi^{(1,j)} := \left(\alpha_{1,i} - \alpha_{1,j}\right)^{-1} P^{(j)} \left(T^{(4)} + T^{(3)}\Xi^{(1,\perp)}\right) P^{(i)} \tag{21}$$

So far no requirement is imposed to $\psi_1^{(i)}$.

Now multiply (17) by Q,

$$H_e\psi_2^{\perp} + QT^{(4)}\psi_0 + QT^{(3)}\psi_1 = \alpha_{1,i}A_e^2\psi_1^{\perp} \tag{22}$$

Since

$$\begin{aligned} QT^{(3)}\psi_1 &= QT^{(3)}\psi_1^{\perp} + \sum_{l\neq i} QT^{(3)}\psi_1^{(l)} + QT^{(3)}\psi_1^{(i)} \\ &= QT^{(3)}\Xi^{(1,\perp)}\psi_0 + \sum_{l\neq i} QT^{(3)}\Xi^{(1,l)}\psi_0 + QT^{(3)}\psi_1^{(i)} \end{aligned}$$

(22) yields

$$H_e\psi_2^{\perp} = -QT^{(4)}\psi_0 + \alpha_{1,i}A_e^2\Xi^{(1,\perp)}\psi_0 - QT^{(3)}\Xi^{(1,\perp)}\psi_0 - \sum_{l\neq i} QT^{(3)}\Xi^{(1,l)}\psi_0 - QT^{(3)}\psi_1^{(i)}$$

Therefrom we obtain

$$\psi_2^{\perp} = \Xi^{(2,\perp)}\psi_0 + \Xi^{(1,\perp)}\psi_1^{(i)}$$

where

$$\Xi^{(2,\perp)} := (H_e)_{\perp}^{-1} \left[\alpha_{1,i}\Xi^{(1,\perp)}A_e^2 - QT^{(3)}\left(\Xi^{(1,\perp)} + \sum_{l\neq i}\Xi^{(1,l)}\right) - QT^{(4)}\right]$$

Third-order:

$$H_e\psi_3 + T^{(3)}\psi_2 + T^{(4)}\psi_1 + T^{(5)}\psi_0 = \mathcal{E}_3A_e^2\psi_0 + \alpha_{2,i}A_e^2\psi_1 + \alpha_{1,i}A_e^2\psi_2 \tag{23}$$

Multiply by $P^{(j)}$, rearrange terms, and use (19) to obtain

$$\begin{aligned} \mathcal{E}_3P^{(j)}\psi_0 &= P^{(j)}T^{(3)}\psi_2 + P^{(j)}T^{(4)}\psi_1 + P^{(j)}T^{(5)}\psi_0 - \alpha_{2,i}\psi_1^{(j)} - \alpha_{1,i}\psi_2^{(j)} \\ &= P^{(j)}T^{(3)}\left(\psi_2^{\perp} + \psi_2^{||}\right) + P^{(j)}T^{(4)}\left(\psi_1^{\perp} + \sum_{l\neq i}\psi_1^{(l)} + \psi_1^{(i)}\right) \\ &\quad + P^{(j)}T^{(5)}\psi_0 - \alpha_{2,i}\psi_1^{(j)} - \alpha_{1,i}\psi_2^{(j)} \\ &= P^{(j)}T^{(3)}\psi_2^{\perp} + P^{(j)}T^{(4)}\left(\psi_1^{\perp} + \sum_{l\neq i}\psi_1^{(i)} + \psi_1^{(i)}\right) \\ &\quad + P^{(j)}T^{(5)}\psi_0 - \left(\alpha_{1,i} - \alpha_{1,j}\right)\psi_2^{(j)} - \alpha_{2,i}\psi_1^{(j)} \end{aligned} \tag{24}$$

For $j = i$ we have

$$\begin{aligned}
\mathcal{E}_3\psi_0 &= P^{(i)}T^{(3)}\Xi^{(2,\perp)}\psi_0 + P^{(i)}T^{(4)}\left(\Xi^{(1,\perp)} + \sum_{l\neq i}\Xi^{(1,l)}\right)\psi_0 + P^{(i)}T^{(5)}\psi_0 \\
&\quad + P^{(i)}T^{(3)}\Xi^{(1,\perp)}\psi_1^{(i)} + P^{(i)}T^{(4)}\psi_1^{(i)} - \alpha_{2,i}\psi_1^{(i)}
\end{aligned}$$

Let us note that

$$P^{(i)}T^{(4)}\psi^{(i)} + P^{(i)}T^{(3)}\Xi^{(1,\perp)}\psi^{(i)} = \Lambda^{(2,i)}\psi^{(i)} = \alpha_{2,i}\psi^{(i)}$$

Thus we obtain $\mathcal{E}_3\psi_0 = \Lambda^{(3,i)}\psi_0$, where

$$\Lambda^{(3,i)} := P^{(i)}\left[T^{(5)} + T^{(4)}\left(\Xi^{(1,\perp)} + \sum_{l\neq i}\Xi^{(1,l)}\right) + T^{(3)}\Xi^{(2,\perp)}\right]P^{(i)}$$

By assumption $\Lambda^{(3,i)}$ has only one eigenvalue $\alpha_{3,i}$ so $\mathcal{E}_3 = \alpha_{3,i}$.

Now for $j \neq i$ we can rewrite (24) as

$$\begin{aligned}
\left(\alpha_{1,i} - \alpha_{1,j}\right)\psi_2^{(j)} &= P^{(j)}T^{(5)}\psi_0 + P^{(j)}T^{(4)}\left(\Xi^{(1,\perp)} + \sum_{l\neq i}\Xi^{(1,l)}\right)\psi_0 \\
&\quad + P^{(j)}T^{(3)}\Xi^{(2,\perp)}\psi_0 - \alpha_{2,i}\Xi^{(1,j)}\psi_0 + P^{(j)}T^{(3)}\Xi^{(1,\perp)}\psi_1^{(i)} + P^{(j)}T^{(4)}\psi_1^{(i)}
\end{aligned}$$

Now use (21) and define

$$\Xi^{(2,j)} := \left(\alpha_{1,i} - \alpha_{1,j}\right)^{-1}P^{(j)}\left[T^{(5)} + T^{(4)}\left(\Xi^{(1,\perp)} + \sum_{l\neq i}\Xi^{(1,l)}\right) + T^{(3)}\Xi^{(2,\perp)} - \alpha_{2,i}\Xi^{(1,j)}\right]P^{(i)}$$

to obtain

$$\psi_2^{(j)} = \Xi^{(2,j)}\psi_0 + \Xi^{(1,j)}\psi_1^{(i)}$$

The last step is to multiply (23) by Q,

$$H_e\psi_3^{\perp} = Q\left(\alpha_{1,i}A_e^2 - T^{(3)}\right)\psi_2 + Q\left(\alpha_{2,i}A_e^2 - T^{(4)}\right)\psi_1 - QT^{(5)}\psi_0 \tag{25}$$

We have

$$\begin{aligned}
Q\left(\alpha_{1,i}A_e^2 - T^{(3)}\right)\psi_2 &= Q\left(\alpha_{1,i}A_e^2 - T^{(3)}\right)\psi_2^{\perp} + \alpha_{1,i}A_e^2 Q\psi_2^{\|} - QT^{(3)}\sum_{l\neq i}\psi_2^{(l)} - QT^{(3)}\psi_2^{(i)} \\
&= Q\left(\alpha_{1,i}A_e^2 - T^{(3)}\right)\Xi^{(2,\perp)}\psi_0 + Q\left(\alpha_{1,i}A_e^2 - T^{(3)}\right)\Xi^{(1,i)}\psi_1^{(i)} \\
&\quad - QT^{(3)}\sum_{l\neq i}\Xi^{(2,l)}\psi_0 - QT^{(3)}\sum_{l\neq i}\Xi^{(1,l)}\psi_1^{(i)} - QT^{(3)}\psi_2^{(i)} \\
&= Q\left[\left(\alpha_{1,i}A_e^2 - T^{(3)}\right)\Xi^{(2,\perp)} - \sum_{l\neq i}T^{(3)}\Xi^{(2,l)}\right]\psi_0 \\
&\quad + Q\left[\left(\alpha_{1,i}A_e^2 - T^{(3)}\right)\Xi^{(1,\perp)} - \sum_{l\neq i}T^{(3)}\Xi^{(1,l)}\right]\psi_1^{(1)} - QT^{(3)}\psi_2^{(i)}
\end{aligned} \tag{26}$$

and similarly

$$Q\left(\alpha_{2,i}A_e^2 - T^{(4)}\right)\psi_1 = Q\left[\left(\alpha_{2,i}A_e^2 - T^{(4)}\right)\Xi^{(1,\perp)} - \sum_{l\neq i} T^{(4)}\Xi^{(1,l)}\right]\psi_0 - QT^{(4)}\psi_1^{(i)} \tag{27}$$

Insert (26) and (27) in (25) and multiply the whole equation by $(H_e)_\perp^{-1}$ to obtain

$$\psi_3^\perp = \Xi^{(3,\perp)}\psi_0 + \Xi^{(2,\perp)}\psi_1^{(i)} + \Xi^{(1,\perp)}\psi_2^{(i)}$$

with

$$\begin{aligned}\Xi^{(3,\perp)} &:= (H_e)_\perp^{-1}\Big[\left(\alpha_{1,i}\Xi^{(2,\perp)} + \alpha_{2,i}\Xi^{(1,\perp)}\right)A_e^2 - QT^{(5)} \\ &\quad - QT^{(4)}\left(\Xi^{(1,\perp)} + \sum_{l\neq i}\Xi^{(1,l)}\right) - QT^{(5)}\left(\Xi^{(2,\perp)} + \sum_{l\neq i}\Xi^{(2,l)}\right)\Big]\end{aligned}$$

As before, one can guess the solution for arbitrary n. Let us summarize hypotheses and results:

Proposition 2 *Define*

$$\begin{aligned}\Lambda^{(1)} &:= PT^{(3)}P \\ \Xi^{(1,\perp)} &:= -(H_e)_\perp^{-1}QT^{(3)}\end{aligned}$$

Suppose that $\Lambda^{(1)}$ has k distinct eigenvalues $\alpha_{1,1},\ldots,\alpha_{1,k}$ with eigenspaces $B_1,\ldots,B_k$. Let $P^{(1)},\ldots,P^{(k)}$ be the associated projection operators. Given $1 \le i \le k$, set

$$\begin{aligned}\Lambda^{(2,i)} &:= P^{(i)}\left(T^{(4)} + T^{(3)}\Xi^{(1,\perp)}\right)P^{(i)} \\ \Xi^{(1,j)} &:= (\alpha_{1,i} - \alpha_{1,j})^{-1}P^{(j)}\left(T^{(4)} + T^{(3)}\Xi^{(1,\perp)}\right)P^{(i)} \\ \Xi^{(2,\perp)} &:= (H_e)_\perp^{-1}\left[\alpha_{1,i}\Xi^{(1,\perp)}A_e^2 - QT^{(4)} - QT^{(3)}\left(\Xi^{(1,\perp)} + \sum_{l\neq i}\Xi^{(1,l)}\right)\right]\end{aligned}$$

and then recursively define

$$\begin{aligned}\Lambda^{(n,i)} &:= P^{(i)}\left(T^{(n+2)} + \sum_{s=1}^{n-1}T^{(n+2-s)}\Xi^{(s,\perp)} + \sum_{s=1}^{n-2}\sum_{l\neq i}T^{(n+2-s)}\Xi^{(s,l)}\right)P^{(i)} \\ \Xi^{(n-1,j)} &:= (\alpha_{1,i} - \alpha_{1,j})^{-1}P^{(j)}\Bigg(T^{(n+2)} + \sum_{s=1}^{n-1}T^{(n+2-s)}\Xi^{(s,\perp)} \\ &\quad + \sum_{s=1}^{n-2}\sum_{l\neq i}T^{(n+2-s)}\Xi^{(s,l)} - \sum_{s=2}^{n-1}\alpha_{s,i}\Xi^{(n-s,j)}\Bigg)P^{(i)} \\ \Xi^{(n,\perp)} &:= (H_e)_\perp^{-1}\left[\sum_{s=1}^{n-1}\alpha_{s,i}\Xi^{(n-s,\perp)}A_e^2 - QT^{(n+2)} - \sum_{s=1}^{n-1}QT^{(s+2)}\left(\Xi^{(n-s,\perp)} + \sum_{l\neq i}\Xi^{(n-s,l)}\right)\right]\end{aligned}$$

where $\alpha_{s,i}$ is (by assumption) the unique eigenvalue of $\Lambda^{(s,i)}$.

Let $\mathcal{E}_n, \psi_n$ be the R-S coefficients. Then $\mathcal{E}_1$ has to be equal to one of the eigenvalues of $\Lambda^{(1)}$, let us say $\mathcal{E}_1 = \alpha_{1,i}$. Consequently, $\psi_0 \in B_i$ and

$$\begin{aligned}
\mathcal{E}_n &= \alpha_{n,i} && (28)\\
\psi_n^{(j)} &= \Xi^{(n,j)}\psi_0 + \sum_{s=1}^{n-1} \Xi^{(n-s,j)}\psi_s^{(i)} && (29)\\
\psi_n^{\perp} &= \Xi^{(n,\perp)}\psi_0 + \sum_{s=1}^{n-1} \Xi^{(n-s,\perp)}\psi_s^{(i)} && (30)\\
\psi_n &= \psi_n^{\perp} + \sum_{j\neq i} \psi_n^{(j)} + \psi_n^{(i)}
\end{aligned}$$

The vectors $\psi_1^{(i)}, \ldots, \psi_n^{(i)}$ are arbitrarily chosen from B_i.

Proof. Use mathematical induction. Because of the discussion above, we only have to prove the inductive step. Thus, let us assume that $\mathcal{E}_m$, $\psi_{m-1}^{(j)}$ and $\psi_m^{\perp}$ are given by (28)–(30), for $m = 2, \ldots, n$. Let us compute $\mathcal{E}_{n+1}$, $\psi_n^{(j)}$ and $\psi_{n+1}^{\perp}$. The $(n+1)$-st order equation is

$$H_e\psi_{n+1} + \sum_{p=0}^{n} T^{(n+3-p)}\psi_p = \sum_{s=0}^{n} \mathcal{E}_{n+1-s}A_e^2\psi_s \qquad (31)$$

We have

$$\begin{aligned}
\sum_{p=0}^{n} T^{(n+3-p)}\psi_p &= T^{(n+3)}\psi_0 + \sum_{p=1}^{n} T^{(n+3-p)}\psi_p^{\perp} + \sum_{p=1}^{n} T^{(n+3-p)} \sum_{l\neq i} \psi_p^{(l)} + \sum_{p=1}^{n} T^{(n+3-p)}\psi_p^{(i)}\\
&= T^{(n+3)}\psi_0 + T^{(n+2)}\Xi^{(1,\perp)}\psi_0 + \sum_{p=2}^{n} T^{(n+3-p)} \left(\Xi^{(p,\perp)}\psi_0 + \sum_{s=1}^{p-1} \Xi^{(p-s,\perp)}\psi_s^{(i)}\right)\\
&\quad + \sum_{l\neq i} T^{(n+2)}\Xi^{(1,l)}\psi_0 + \sum_{p=2}^{n-1}\sum_{l\neq i} T^{(n+3-p)} \left(\Xi^{(p,l)}\psi_0 + \sum_{s=1}^{p-1} \Xi^{(p-s,l)}\psi_s^{(i)}\right)\\
&\quad + \sum_{l\neq i} T^{(3)}\psi_n^{(l)} + \sum_{p=1}^{n} T^{(n+3-p)}\psi_p^{(i)}\\
&= \left(T^{(n+3)} + \sum_{p=1}^{n} T^{(n+3-p)}\Xi^{(p,\perp)} + \sum_{p=1}^{n-1}\sum_{l\neq i} T^{(n+3-p)}\Xi^{(p,l)}\right)\psi_0\\
&\quad + \sum_{s=1}^{n-1}\sum_{p=s+1}^{n} T^{(n+3-p)}\Xi^{(p-s,\perp)}\psi_s^{(i)} + \sum_{s=1}^{n-2}\sum_{p=s+1}^{n-1}\sum_{l\neq i} T^{(n+3-p)}\Xi^{(p-s,l)}\psi_s^{(i)}\\
&\quad + \sum_{l\neq i} T^{(3)}\psi_n^{(l)} + \sum_{s=1}^{n} T^{(n+3-s)}\psi_s^{(i)}
\end{aligned}$$

$$
\begin{aligned}
= \quad & \left(T^{(n+3)} + \sum_{p=1}^{n} T^{(n+3-p)} \Xi^{(p,\perp)} + \sum_{p=1}^{n-1} \sum_{l \neq i} T^{(n+3-p)} \Xi^{(p,l)} \right) \psi_0 \\
& + \sum_{s=1}^{n-1} \sum_{m=1}^{n-s} T^{(n+3-s-m)} \Xi^{(m,\perp)} \psi_s^{(i)} + \sum_{s=1}^{n-2} \sum_{m=1}^{n-1-s} \sum_{l \neq i} T^{(n+3-s-m)} \Xi^{(m,l)} \psi_s^{(i)} \\
& + \sum_{l \neq i} T^{(3)} \psi_n^{(l)} + \sum_{s=1}^{n} T^{(n+3-s)} \psi_s^{(i)}
\end{aligned}
$$

where we use that $\sum_{p=1}^{r} \sum_{s=1}^{p-1} F_{sp} = \sum_{s=1}^{r-1} \sum_{p=s+1}^{r} F_{sp}$ and then we change index $p \to m = p - s$.

Let us multiply (31) by $P^{(i)}$. Since $P^{(i)} H_e = 0$ and $P^{(i)} A_e^2 = A_e^2 P^{(i)} = P^{(i)}$, we obtain

$$
\sum_{p=0}^{n} P^{(i)} T^{(n+3-p)} \psi_p = \mathcal{E}_{n+1} \psi_0 + \sum_{s=1}^{n} \alpha_{n+1-s,i} \psi_s^{(i)} \tag{32}
$$

The left-hand side can be written as

$$
\begin{aligned}
\sum_{p=0}^{n} P^{(i)} T^{(n+3-p)} \psi_p \quad = \quad & P^{(i)} \left(T^{(n+3)} + \sum_{p=1}^{n} T^{(n+3-p)} \Xi^{(p,\perp)} + \sum_{p=1}^{n-1} \sum_{l \neq i} T^{(n+3-p)} \Xi^{(p,l)} \right) \psi_0 \\
& + \sum_{s=1}^{n-2} P^{(i)} \left(T^{(n+3-s)} + \sum_{m=1}^{n-s} T^{(n+3-s-m)} \Xi^{(m,\perp)} \right. \\
& + \left. \sum_{m=1}^{n-1-s} \sum_{l \neq i} T^{(n+3-s-m)} \Xi^{(m,l)} \right) \psi_s^{(i)} \\
& + P^{(i)} \left(T^{(3)} \Xi^{(1,\perp)} + T^{(4)} \right) \psi_{n-1}^{(i)} + \sum_{l \neq i} P^{(i)} T^{(3)} \psi_n^{(l)} + P^{(i)} T^{(3)} \psi_n^{(i)}
\end{aligned}
$$

By the argument used in (19), we see that $\sum_{l \neq i} P^{(i)} T^{(3)} \psi_n^{(l)} = 0$. Also $\psi_s^{(i)} = P^{(i)} \psi_s^{(i)}$. Then

$$
\sum_{p=0}^{n} P^{(i)} T^{(n+3-p)} \psi_p = \Lambda^{(n+1,i)} \psi_0 + \sum_{s=1}^{n} \Lambda^{(n+1-s,i)} \psi_s^{(i)} \tag{33}
$$

Inserting (33) into (32) we conclude

$$
\Lambda^{(n+1,i)} \psi_0 = \mathcal{E}_{n+1} \psi_0
$$

Now let us multiply (31) by $P^{(j)}$ for $j \neq i$. Since $P^{(j)} \psi_0 = 0$, we have

$$
\alpha_{1,i} \psi_n^{(j)} = \sum_{p=0}^{n} P^{(j)} T^{(n+3-p)} \psi_p - \sum_{s=1}^{n-1} \alpha_{n+1-s,i} \psi_s^{(j)} \tag{34}
$$

The right-hand side can be manipulated in the same way as before. The result is

$$\begin{aligned}\sum_{p=0}^{n} P^{(i)}T^{(n+3-p)}\psi_p - \sum_{s=1}^{n-1}\alpha_{n+1-s,i}\psi_s^{(j)} \\ = (\alpha_{1,i}-\alpha_{1,j})\Xi^{(n,j)}\psi_0 + \sum_{s=1}^{n-1}(\alpha_{1,i}-\alpha_{1,j})\Xi^{(n-s,j)}\psi_s^{(i)} + \sum_{l=1}^{k} P^{(j)}T^{(3)}\psi_n^{(l)}\end{aligned}$$

As proven in (19), the last term above is equal to $\alpha_{1,j}\psi_n^{(j)}$. Thus (34) leads to

$$\psi_n^{(j)} = \Xi^{(n,j)}\psi_0 + \sum_{s=1}^{n-1}\Xi^{(n-s,j)}\psi_s^{(i)}$$

Finally, multiply (31) by Q,

$$H_e\psi_{n+1}^{\perp} = \sum_{p=1}^{n}\alpha_{n+1-p,i}A_e^2\psi_p^{\perp} - \sum_{p=0}^{n} QT^{(n+3-p)}\psi_p \tag{35}$$

For the first term we have

$$\begin{aligned}\sum_{p=1}^{n}\alpha_{n+1-p,i}A_e^2\psi_p^{\perp} &= \sum_{s=1}^{n}\alpha_{n+1-s,i}A_e^2\Xi^{(s,\perp)}\psi_0 + \sum_{p=2}^{n}\sum_{s=1}^{p-1}\alpha_{n+1-p,i}A_e^2\Xi^{(p-s,\perp)}\psi_s^{(i)} \\ &= \sum_{s=1}^{n}\alpha_{n+1-s,i}A_e^2\Xi^{(s,\perp)}\psi_0 + \sum_{s=1}^{n-1}\sum_{m=1}^{n-s}\alpha_{n+1-s-m,i}A_e^2\Xi^{(m,\perp)}\psi_s^{(i)}\end{aligned}$$

and for the second one

$$\begin{aligned}\sum_{p=0}^{n} QT^{(n+3-p)}\psi_p &= Q\left(T^{(n+3)} + \sum_{p=1}^{n} T^{(n+3-p)}\Xi^{(p,\perp)} + \sum_{p=1}^{n-1}\sum_{l\neq i} T^{(n+3-p)}\Xi^{(p,l)}\right)\psi_0 \\ &\quad + \sum_{s=1}^{n-2} Q\left(T^{(n+3-s)} + \sum_{m=1}^{n-s} T^{(n+3-s-m)}\Xi^{(m,\perp)}\right. \\ &\quad \left. + \sum_{m=1}^{n-1-s}\sum_{l\neq i} T^{(n+3-s-m)}\Xi^{(m,l)}\right)\psi_s^{(i)} \\ &\quad + Q\left(T^{(3)}\Xi^{(1,\perp)} + T^{(4)}\right)\psi_{n-1}^{(i)} + \sum_{l\neq i} QT^{(3)}\psi_n^{(l)} + QT^{(3)}\psi_n^{(i)}\end{aligned}$$

Then insert these expressions into (35). After multiplying the whole equation by $(H_e)_{\perp}^{-1}$ we obtain the desired result. $\square$

As before, we set $\psi_n^{(i)} = 0$ for all $n = 1, 2, \ldots$. Consequently, ψ_n will be orthogonal to ψ_0 and

$$\psi_n = \left(\Xi^{(n,\perp)} + \sum_{l\neq i}\Xi^{(n,l)}\right)\psi_0$$

The following expressions will be useful later:

$$\begin{aligned}
\Lambda^{(n,i)}\psi_0 &= P^{(i)}T^{(n+2)}\psi_0 + \sum_{s=1}^{n-2} P^{(i)}T^{(n+2-s)}\psi_s + P^{(i)}T^{(3)}\psi_{n-1}^{\perp} && (36)\\
\psi_n^{\perp} &= (H_e)_{\perp}^{-1}\left[\sum_{s=1}^{n-1}\mathcal{E}_s A_e^2 \psi_{n-s}^{\perp} - QT^{(n+2)}\psi_0 - \sum_{s=1}^{n-1} QT^{(s+2)}\psi_{n-s}\right] && (37)\\
\psi_{n-1}^{(j)} &= (\alpha_{1,i}-\alpha_{1,j})^{-1}\Bigg(P^{(j)}T^{(n+2)}\psi_0 + \sum_{s=1}^{n-2} P^{(j)}T^{(n+2-s)}\psi_s \\
&\quad + P^{(j)}T^{(3)}P_{|j|\le a+3(n-1)}\psi_{n-1}^{\perp} - \sum_{s=2}^{n-1}\mathcal{E}_s\psi_{n-s}^{(j)}\Bigg) && (38)
\end{aligned}$$

Next, let us estimate the growth of these coefficients. Since $\mathcal{E}_n\psi_0 = \Lambda^{(n,i)}\psi_0$,

$$\begin{aligned}
|\mathcal{E}_n| &= \left|\left\langle\psi_0, \Lambda^{(n,i)}\psi_0\right\rangle\right| \\
&\le \left|\left\langle\psi_0, P^{(i)}T^{(n+2)}\psi_0\right\rangle\right| + \sum_{s=1}^{n-2}\left|\left\langle\psi_0, P^{(i)}T^{(n+2-s)}\psi_s\right\rangle\right| + \left|\left\langle\psi_0, P^{(i)}T^{(3)}\psi_{n-1}^{\perp}\right\rangle\right| \\
&\le \left\|T^{(n+2)}P_{|j|\le a}\right\| + \sum_{s=1}^{n-2}\left|\left\langle T^{(n+2-s)}\psi_0, \psi_s\right\rangle\right| + \left|\left\langle T^{(3)}\psi_0, \psi_{n-1}^{\perp}\right\rangle\right| \\
&\le \left\|T^{(n+2)}P_{|j|\le a}\right\| + \sum_{s=1}^{n-2}\left\|T^{(n+2-s)}P_{|j|\le a}\right\|\|\psi_s\| + \left\|T^{(3)}P_{|j|\le a}\right\|\|\psi_{n-1}^{\perp}\| \\
&= \sum_{s=2}^{n}\left\|T^{(s+2)}P_{|j|\le a}\right\|\|\psi_{n-s}\| + \left\|T^{(3)}P_{|j|\le a}\right\|\|\psi_{n-1}^{\perp}\| && (39)
\end{aligned}$$

This calculation follows from (36), the self-adjointness of $T^{(l)}$, and Lemma 1.

It is easy to see that $\|(H_e)_{\perp}^{-1}\| = \|A_e\| = 1$. Then from (37) we have

$$\begin{aligned}
\left\|\psi_n^{\perp}\right\| &\le \sum_{s=1}^{n-1}|\mathcal{E}_s|\left\|\psi_{n-s}^{\perp}\right\| + \left\|T^{(n+2)}P_{|j|\le a}\right\|\|\psi_0\| + \sum_{s=1}^{n-1}\left\|T^{(s+2)}P_{|j|\le a+3(n-s)}\right\|\|\psi_{n-s}\| \\
&= \sum_{s=1}^{n-1}|\mathcal{E}_s|\left\|\psi_{n-s}^{\perp}\right\| + \sum_{s=1}^{n}\left\|T^{(s+2)}P_{|j|\le a+3(n-s)}\right\|\|\psi_{n-s}\| && (40)
\end{aligned}$$

Finally let us consider (38)

$$\begin{aligned}
\left\|\psi_{n-1}^{(j)}\right\| &\le |\alpha_{1,i}-\alpha_{1,j}|^{-1}\Bigg(\left\|T^{(n+2)}P_{|j|\le a}\right\|\|\psi_0\| + \sum_{s=1}^{n-2}\left\|P^{(j)}T^{(n+2-s)}\right\|\|\psi_s\| \\
&\quad + \left\|P^{(j)}T^{(3)}\right\|\left\|\psi_{n-1}^{\perp}\right\| + \sum_{s=2}^{n-1}|\mathcal{E}_s|\left\|\psi_{n-s}^{(j)}\right\|\Bigg)
\end{aligned}$$

Set $D := \min_{j\neq i} |\alpha_{1,i} - \alpha_{1,j}|^{-1}$. Also, let us notice that $\left\|P^{(j)} T^{(n+2-s)}\right\| = \left\|T^{(n+2-s)} P^{(j)}\right\| = \left\|T^{(n+2-s)} P_{|j|\leq a} P^{(j)}\right\| \leq \left\|T^{(n+2-s)} P_{|j|\leq a}\right\|$. Thus

$$\left\|\psi^{(j)}_{n-1}\right\| \leq D \sum_{s=2}^{n-1} |\mathcal{E}_s| \left\|\psi^{(j)}_{n-s}\right\| + D \sum_{s=2}^{n} \left\|T^{(s+2)} P_{|j|\leq a}\right\| \|\psi_{n-s}\| + D \left\|T^{(3)} P_{|j|\leq a}\right\| \left\|\psi^{\perp}_{n-1}\right\| \tag{41}$$

These inequalities will allow us to obtain upper bounds for the growth of R-S coefficients. To do that, we need some technical results.

Lemma 3 *Let $\kappa \geq 2$ be the number defined in Lemma 2. Then*

1. *For each $a \geq 0$ there is a constant γ_a so that, for all $m \geq 0$,*

$$\sum_{l=0}^{m} \left[\frac{(1+a+m-l)!(1+a+l)!}{(1+a+m)!}\right]^{\frac{1}{2}} \leq \gamma_a$$

2. *For all $a \geq -1$ there is a constant β so that, for all $m \geq 0$,*

$$\sum_{l=0}^{m} \kappa^{-\frac{5l}{2}} \left[\frac{(1+a+3m-2l)!(1+a+m-l)!}{(1+a+3m-3l)!(1+a+m)!}\right]^{\frac{1}{2}} \leq \beta$$

3. *For each $a \geq 0$ there is a constant g_a so that, for all $m \geq 0$,*

$$\sum_{l=1}^{m} \kappa^{-\frac{5l}{2}} \left[\frac{(1+a+l)!(1+a+m-l)!}{(1+a)!(a+m)!}\right]^{\frac{1}{2}} \leq g_a$$

Proof. Since $\kappa \geq 2$, it suffices to show the assertions for $\kappa = 2$. Statement 1 and 2 are proven in Lemma 2 of [15]. To show 3, notice that for $1 \leq l \leq m-1$ we have

$$\frac{(1+a+l)!(1+a+m-l)!}{(a+m)!(1+a)!} = (1+a+l)\frac{\prod_{s=1}^{m-l}(1+a+s)}{\prod_{s=l}^{m-1}(1+a+s)} = (1+a+l)\prod_{s=1}^{m-l}\frac{1+a+s}{l+a+s} \leq 1+a+l$$

Therefore

$$\sum_{l=1}^{m} 2^{-\frac{5l}{2}} \left[\frac{(1+a+l)!(1+a+m-l)!}{(a+m)!(1+a)!}\right]^{\frac{1}{2}} \leq \sum_{l=1}^{m} 2^{-\frac{5l}{2}} (1+a+l)^{\frac{1}{2}}$$

where the right-hand side converges to some constant $g_a < \infty$. □

Theorem 2 *Define $b_1 := \gamma\left[k g_a + (2+a)^{\frac{1}{2}}\right]$, $b_2 := 8D\left[b_1\gamma_a + \gamma(2+a)^{\frac{1}{2}} + \gamma k g_a\right]$ and $b_3 := b_1\gamma_a + \gamma\beta[1 + b_2(k-1)]$. Then for any $b \geq \max\{b_1, b_2, b_3, 1\}$ and for $n = 1, 2, \ldots$,*

$$|\mathcal{E}_n| \leq b_1 \kappa^{3n} b^{n-2} \left[(a+n)!\right]^{\frac{1}{2}} \tag{42}$$

$$\left\|\psi^{(l)}_{n-1}\right\| \leq b_2 \kappa^{3(n-1)} b^{n-2} \left[(a+n)!\right]^{\frac{1}{2}} \tag{43}$$

$$\left\|\psi^{\perp}_{n}\right\| \leq b_3 \kappa^{3n} b^{n-2} \left[(1+a+n)!\right]^{\frac{1}{2}} \tag{44}$$

Proof. Assume the estimates are true for $s = 1, \ldots, n-1$. This implies that

$$\|\psi_s\| \leq [1 + b_2(k-1)]\kappa^{3s} b^{s-1}[(1+a+s)!]^{\frac{1}{2}} \leq \kappa^{3s} k b^s [(1+a+s)!]^{\frac{1}{2}} \tag{45}$$

for $s \leq n-2$. We will use the second inequality in (45) to prove (42) and (43), and the first one to prove (44).

Let us start by showing (42). Applying Lemmas 2 and 3 we obtain

$$\begin{aligned}
\sum_{s=2}^{n} \left\|T^{(s+2)} P_{|j|\leq a}\right\| \|\psi_{n-s}\| &\leq \gamma k \sum_{s=2}^{n} \kappa^{\frac{s}{2}} \left[\frac{(1+a+s)!}{(1+a)!}\right]^{\frac{1}{2}} \kappa^{3(n-s)} b^{n-s} [(1+a+n-s)!]^{\frac{1}{2}} \\
&\leq \gamma k \kappa^{3n} b^{n-2} [(a+n)!]^{\frac{1}{2}} \sum_{s=2}^{n} \kappa^{-\frac{5s}{2}} \left[\frac{(1+a+s)!(1+a+n-s)!}{(1+a)!(a+n)!}\right]^{\frac{1}{2}} \\
&\leq \gamma k g_a \kappa^{3n} b^{n-2} [(a+n)!]^{\frac{1}{2}}
\end{aligned}$$

thus (39) yields

$$\begin{aligned}
|\mathcal{E}_n| &\leq \gamma k g_a \kappa^{3n} b^{n-2} [(a+n)!]^{\frac{1}{2}} + \gamma \kappa^{3(n-1)} b_3 b^{n-3} \kappa^{\frac{1}{2}} (2+a)^{\frac{1}{2}} [(a+n)!]^{\frac{1}{2}} \\
&\leq \gamma k g_a \kappa^{3n} b^{n-2} [(a+n)!]^{\frac{1}{2}} + \gamma (2+a)^{\frac{1}{2}} \kappa^{3n} b^{n-2} [(a+n)!]^{\frac{1}{2}} \\
&\leq b_1 \kappa^{3n} b^{n-2} [(a+n)!]^{\frac{1}{2}}
\end{aligned}$$

which completes the proof of (42). To prove (43) we start from (41) and proceed in the same fashion

$$\begin{aligned}
\left\|\psi_{n-1}^{(j)}\right\| &\leq D \kappa^{3n} b_1 b_2 b^{n-3} \sum_{s=2}^{n-1} [(a+s)!(1+a+n-s)!]^{\frac{1}{2}} + D\gamma \kappa^{3n} b_3 b^{n-3} (2+a)^{\frac{1}{2}} [(a+n)!]^{\frac{1}{2}} \\
&\quad + D\gamma k \kappa^{3n} b^{n-2} \sum_{s=2}^{n} \kappa^{-\frac{5s}{2}} \left[\frac{(1+a+s)!(1+a+n-s)!}{(1+a)!}\right]^{\frac{1}{2}} \\
&\leq D b_1 \kappa^{3n} b^{n-2} [(a+n)!]^{\frac{1}{2}} \sum_{m=1}^{n-2} \left[\frac{(1+a+m)!(a+n-m)!}{(a+n)!}\right]^{\frac{1}{2}} \\
&\quad + D\gamma (2+a)^{\frac{1}{2}} \kappa^{3n} b^{n-2} [(a+n)!]^{\frac{1}{2}} \\
&\quad + D\gamma k \kappa^{3n} b^{n-2} [(a+n)!]^{\frac{1}{2}} \sum_{s=2}^{n} \kappa^{-\frac{5s}{2}} \left[\frac{(1+a+s)!(1+a+n-s)!}{(1+a)!(a+n)!}\right]^{\frac{1}{2}}
\end{aligned}$$

where we have changed index $s \to m = s-1$ in the first term. From this and statements 1 and 3 of Lemma 3, we obtain

$$\begin{aligned}
\left\|\psi_{n-1}^{(j)}\right\| &\leq 8D \left[b_1 \gamma_a + \gamma (2+a)^{\frac{1}{2}} + \gamma k g_a\right] \kappa^{3(n-1)} b^{n-2} [(a+n)!]^{\frac{1}{2}} \\
&= b_2 \kappa^{3(n-1)} b^{n-2} [(a+n)!]^{\frac{1}{2}}
\end{aligned}$$

so (43) is done. Consequently, (45) must be valid for $s = n - 1$.

Finally let us show (44). Note that the first term of (40) is bounded like the first term of (41). Applying statement 2 of Lemma 3, it follows that

$$\begin{aligned}
\left\|\psi_n^{\perp}\right\| &\leq b_1 b_3 \kappa^{3n} b^{n-3} g_a [(a+n)!]^{\frac{1}{2}} \\
&\quad + \gamma[1 + b_2(k-1)]\kappa^{3n} b^{n-2}[(1+a+n)!]^{\frac{1}{2}} \sum_{s=1}^{n} \kappa^{-\frac{5s}{2}} \left[\frac{(1+a+3n-2s)!(1+a+n-s)!}{(1+a+3n-3s)!(1+a+n)!}\right]^{\frac{1}{2}} \\
&\leq b_1 g_a \kappa^{3n} b^{n-2}[(1+a+n)!]^{\frac{1}{2}} + \gamma[1+b_2(k-1)]\beta\kappa^{3n} b^{n-2}[(1+a+n)!]^{\frac{1}{2}} \\
&= b_3 \kappa^{3n} b^{n-2}[(1+a+n)!]^{\frac{1}{2}}
\end{aligned}$$

□

Corollary 1

$$\begin{aligned}
|\mathcal{E}_n| &\leq \kappa^{3n} b^{n-1} [(a+n)!]^{\frac{1}{2}} \\
\|\psi_n\| &\leq \kappa^{3n} k b^{n} [(1+a+n)!]^{\frac{1}{2}}
\end{aligned}$$

For the case where degeneracy is partly broken only up to second order, one needs to define certain operators $\Lambda^{(n,i_1,i_2)}$, $\Xi^{(n-2,i_1,i_2)}$, $\Xi^{(n,\perp)}$ for $n \geq 3$, in addition to those already defined in the last subsection. Now ψ_0 would be required to lie in a certain subspace $B_{i_1,1_2} \in B_{i_1} \in B$, and one would be able to determine ψ_n module an arbitrary component in $B_{i_1,1_2}$. This scheme may be extended to the general case. But the complexity of the set of equations that recursively defines those operators rapidly becomes wild. For that reason, we do not go further. We assume instead that, in general,

$$\begin{aligned}
|\mathcal{E}_n| &\leq \kappa^{3n} b^{n+w} [(1+a+n)!]^{\frac{1}{2}} \\
\|\psi_n\| &\leq \kappa^{3n} b^{n+w} [(1+a+n)!]^{\frac{1}{2}}
\end{aligned}$$

for some positive integer w, which may depend on where degeneracy splits.

4 The two-side error function

Our upper bounds for $|\mathcal{E}_n|$ and $\|\psi_n\|$ will allows us to estimate the error made in the Schrödinger equation when truncated series are inserted in it. We just mimic the technique developed in [15], which is inspired by [3].

For $N \geq 1$ define

$$E_N = e + \sum_{n=1}^{N-1} \hbar^{\frac{n}{2}} \mathcal{E}_n \qquad \Psi_N(x) = \psi_0(x) + \sum_{n=1}^{N-1} \hbar^{\frac{n}{2}} \psi_n(x)$$

These are the truncation at order N of the R-S series. Then define

$$\begin{aligned}\xi_N(x) &= A_e\left[H_0 + W(\hbar;x) - E_N\right]A_e\Psi_N(x) \\ &= \left[H_e + A_eW(\hbar;x)A_e - \sum_{j=1}^{N-1}\hbar^{\frac{j}{2}}\mathcal{E}_jA_e^2\right]\sum_{m=0}^{N-1}\hbar^{\frac{m}{2}}\psi_m(x) \qquad (46)\end{aligned}$$

We call $\xi_N(x)$ the two-side error function since it is the difference between both sides of the Schrödinger equation when exact eigenvalues and eigenfunctions are replaced by truncated series. It can be portrayed in a more suitable way through a huge number of cancellations. This calculation is outlined in the appendix. The result is

$$\xi_N(x) = \sum_{n=0}^{N-1}\hbar^{\frac{n}{2}}A_eW^{[N-n+1]}(\hbar;x)A_e\psi_n(x) - \sum_{n=N}^{2N-2}\hbar^{\frac{n}{2}}\sum_{j=n-N+1}^{N-1}\mathcal{E}_jA_e^2\psi_{m-j}(x)$$

where $W^{[j]}(\hbar;x)$ is the tail of the Taylor series of $V(\hbar;x)$

$$W^{[j]}(\hbar;x) = V(\hbar;x) - \sum_{l=2}^{j}\hbar^{\frac{l-2}{2}}\sum_{|m|=l}\frac{D^mV(0)}{m!}x^m = \hbar^{\frac{j-1}{2}}\sum_{|m|=j+1}\frac{D^mV\left(\zeta_j\right)}{m!}x^m$$

where $\zeta_j = \zeta_j(x) = \Theta_jx$ with $\Theta_j \in (0,1)$, as the Taylor theorem states. So we have

$$\xi_N(x) = \hbar^{\frac{N}{2}}\sum_{n=0}^{N-1}\sum_{|m|=N-n+2}\frac{D^mV\left(\zeta_n\right)}{m!}A_ex^mA_e\psi_n(x) - \sum_{n=N}^{2N-2}\hbar^{\frac{n}{2}}\sum_{l=n-N+1}^{N-1}\mathcal{E}_lA_e^2\psi_{n-l}(x) \qquad (47)$$

Our main result in the next section relies on an upper bound of norm of $(H-E_N)A_e\psi_N = A_e^{-1}\xi_N$. Note that although A_e^{-1} is unbounded, ξ_N is in its domain. To estimate the norm of $A_e^{-1}\xi_N$, we first set a suitable closed region around $x=0$. Then we compute that norm inside and outside of that region. Most of the work is involved in the outside estimate, which requires control on the growth of derivatives of $V(x)$ far away from the minimum of $V(x)$. That is done by resorting to the Cauchy integral formula and hypothesis H2.

Let $\zeta = (\zeta_1,\ldots,\zeta_d) \in \mathbb{R}^d$. Let Γ_i be a circle of radius δ in the complex plane, centered at ζ_i. Then the Cauchy integral formula applied to $V(x)$, which makes sense because of hypothesis H2, states that for each $m = (m_1,\ldots,m_d)$

$$D^mV(\zeta) = \frac{m!}{(2\pi i)^d}\int_{\Gamma_1}dz_1\ldots\int_{\Gamma_d}dz_d\,\frac{V(z)}{\prod_{i=1}^{d}\left(z_i-\zeta_i\right)^{m_i+1}}$$

which implies

$$\frac{\delta^{|m|}}{m!}\left|D^mV(\zeta)\right| \leq K\exp\left(2\tau|\zeta|^2\right) \qquad (48)$$

where we define $K := M\exp\left(2\tau d\delta^2\right)$.

The following lemma states the key result need in the estimate of $\|A_e^{-1}\xi_N\|$. First, let us define

$$\chi_R(x) = \begin{cases} 1 & \text{if } \sum_i^d \omega_i x_i^2 \le R^2 \\ 0 & \text{otherwise.} \end{cases}$$

Lemma 4 *Set $R = \sqrt{6N+2a+d-4}$. Given $m = (m_1, \ldots, m_d)$ with $|m| \ge 2$, and $n = 0, \ldots, N-1$, there are certain constants F and G so that*

$$\left\| \frac{\delta^{|m|}}{m!} D^m V(\zeta) x^{m'} \left(1-\chi_R\right) P_{|j|\le a+3n+1} \right\| \le F G^{\frac{3n+2+a}{2}} \frac{(3n+a+d)^{\frac{d-1}{2}}}{\left(1-\frac{\tau}{\omega_0}\right)^{\frac{|m|}{2}}} \left[\frac{(3n+|m|+[\![d/2]\!]+a)!}{(3n+a)!}\right]^{\frac{1}{2}}$$

where $|m'| = |m|-1$, $\omega_0 = \min\{\omega_1, \ldots, \omega_d\}$, and $[\![\alpha]\!]$ stands for the largest integer less or equal to α.

Proof. Since $|\zeta| \le |x|$, (48) implies

$$\frac{\delta^{|m|}}{m!} \left|D^m V(\zeta)\right| \le K \exp\left(2\tau |x|^2\right) \tag{49}$$

Let us consider an eigenfuction $\Phi_j(x)$ of H_0. For these functions

$$\begin{aligned} \left\| \frac{\delta^{|m|}}{m!} D^m V(\zeta) x^{m'} \left(1-\chi_R\right) \Phi_j(x) \right\|^2 &= \int \left| \frac{\delta^{|m|}}{m!} D^m V(\zeta) \right|^2 x^{2m'} \left|\Phi_j(x)\right|^2 \left[1-\chi_R(x)\right] d^d x \\ &\le K^2 \int e^{4\tau|x|^2} x^{2m'} \left|\Phi_j(x)\right|^2 \left[1-\chi_R(x)\right] d^d x \end{aligned}$$

The inequality comes from (49). Now change variables $x_i \to y_i = \sqrt{\omega_i} x_i$ to get

$$\begin{aligned} \left\| \frac{\delta^{|m|}}{m!} D^m V(\zeta) x^{m'} \left(1-\chi_R\right) \Phi_j(x) \right\|^2 &\le K^2 \left(\prod_{i=1}^d \omega_i^{-m_i'-\frac{1}{2}}\right) \int e^{\sum_i 4\frac{\tau}{\omega_i} y_i^2} y^{2m'} \left|\Phi_j(y)\right|^2 \left[1-\chi_R(y)\right] d^d y \\ &\le K^2 \left(\prod_{i=1}^d \omega_i^{-m_i'-\frac{1}{2}}\right) \int e^{4\frac{\tau}{\omega_0}|y|^2} y^{2m'} \left|\Phi_j(y)\right|^2 \left[1-\chi_R(y)\right] d^d y \\ &= F_1 \left\| e^{2\frac{\tau}{\omega_0}|y|^2} y^{m'} \left(1-\chi_R\right) \Phi_j(y) \right\|^2 \end{aligned} \tag{50}$$

where ω_0 is the lowest eigenfrequency of H_0 and F_1 is defined in the obvious way. In the new variables

$$\chi_R(y) = \begin{cases} 1 & \text{if } y^2 \le R^2 \\ 0 & \text{otherwise.} \end{cases}$$

Using the new variables in (5), we see that $\Phi_j(y)$ is an eigenfunction of the normalized harmonic oscillator operator

$$H_0' = -\frac{1}{2}\Delta_y + \frac{1}{2} y^2$$

with energy $e_j = |j| + d/2$. For $d \geq 2$ this operator is equal to

$$H_0' = \frac{1}{2}\left(-\frac{\partial^2}{\partial r^2} - \frac{d-1}{r}\frac{\partial}{\partial r} + \frac{\mathcal{L}^2}{r^2} + r^2\right)$$

in spherical coordinates, where $\mathcal{L}^2$ is the angular momentum operator defined on S^{d-1}. The eigenvalues now read $e = 2n + q + d/2$ and the eigenfunctions are

$$\Psi_{k,q,\nu}(r,\omega) = \left[\frac{2k!}{\Gamma\left(k+q+\frac{d}{2}\right)}\right]^{\frac{1}{2}} r^q L_k^{q+\frac{d}{2}-1}\left(r^2\right)\exp\left(-\frac{r^2}{2}\right) Y_{q,\nu}(\omega)$$

Here $Y_{q,\nu}(\omega)$ are the normalized eigenfunctions of $\mathcal{L}^2$, with quantum numbers q, ν. For each $q = 0, 1, \ldots$ there are ν_q values of ν. Although the explicit formula for ν_q is rather clumsy, there is a simple bound for it, namely $\nu_q \leq C_d e^{\alpha_d q}$. This bound suffices for the purpose of our proof. $L_k^\beta(x)$ denotes the Laguerre polynomial. By Lemma 6.2 of [3], this polynomial satisfies $\left|L_n^{q+\frac{d}{2}-1}(x)\right| \leq \frac{x^k}{k!}$ for all $x > 4k + 2q + d$. Finally, by equating the expressions for the energy we obtain $|j| = 2k + q$.

Now $\Phi_j(y)$ is certain linear combination of $\Psi_{k,q,\nu}(r,\omega)$,

$$\Phi_j(y) = \sum_{\substack{k,q,\nu: \\ 2k+q=|j|}} c_{k,q,\nu}\Psi_{k,q,\nu}(r,\omega)$$

with $\sum |c_{k,q,\nu}|^2 = 1$. Inserting this linear conbination into (50) and using the Hölder inequality, it follows that

$$\begin{aligned}
&\left\|\frac{\delta^{|m|}}{m!} D^m V(\zeta) x^{m'}\left(1-\chi_R\right)\Phi_j(x)\right\|^2 \\
&\qquad \leq \; F_1 \sum_{\substack{k,q,\nu: \\ 2k+q=|j|}} \left\| e^{2\frac{\tau}{\omega_0}y^2} y^{m'}\left(1-\chi_R\right)\Psi_{k,q,m}(y)\right\|^2 \\
&\qquad \leq \; F_1 \sum_{\substack{k,q,\nu: \\ 2k+q=|j|}} \frac{2k! A_{d-1}}{\Gamma\left(k+q+\frac{d}{2}\right)} \int_R^\infty e^{-\left(1-\frac{4\tau}{\omega_0}\right)r^2} r^{2(|m|-1+q)} \left|L_k^{q+\frac{d}{2}-1}\left(r^2\right)\right|^2 r^{d-1} dr
\end{aligned}$$

where A_{d-1} is the area of the $(d-1)$ dimensional unit sphere. We also have used that $y^{2|m'|} \leq r^{2|m'|} = r^{2(|m|-1)}$. Since $R \geq \sqrt{2|j| + d}$, Lemma 6.2 of [3] applies so

$$\begin{aligned}
&\left\|\frac{\delta^{|m|}}{m!} D^m V(\zeta) x^{m'}\left(1-\chi_R\right)\Phi_j(x)\right\|^2 \\
&\qquad \leq \; F_1 \sum_{\substack{k,q,\nu: \\ 2k+q=|j|}} \frac{2A_{d-1}}{k!\Gamma\left(k+q+\frac{d}{2}\right)} \int_R^\infty e^{-\left(1-\frac{4\tau}{\omega_0}\right)r^2} r^{2|m|+2q+4k+d-3)} dr
\end{aligned}$$

$$
\begin{aligned}
&= F_1 \sum_{\substack{k,q,\nu:\\ 2k+q=|j|}} \frac{2A_{d-1}}{k!\Gamma\left(k+q+\frac{d}{2}\right)} \frac{\Gamma\left(|m|+q+2k+\frac{d}{2}-1\right)}{2\left(1-\frac{4\tau}{\omega_0}\right)^{|m|+q+2k+\frac{d}{2}-1}} \\
&= F_1 A_{d-1} \frac{\Gamma\left(|m|+|j|+\frac{d}{2}-1\right)}{\left(1-\frac{4\tau}{\omega_0}\right)^{|m|+|j|+\frac{d}{2}-1}} \sum_{\substack{k,q:\\ 2k+q=|j|}} \frac{\nu_q}{k!\Gamma\left(k+q+\frac{d}{2}\right)} \\
&= F_1 A_{d-1} \frac{\Gamma\left(|m|+|j|+\frac{d}{2}-1\right)}{\left(1-\frac{4\tau}{\omega_0}\right)^{|m|+|j|+\frac{d}{2}-1}} \sum_{k=0}^{\left[\!\left[\frac{|j|}{2}\right]\!\right]} \frac{\nu_{|j|-2k}}{k!\Gamma\left(|j|-k+\frac{d}{2}\right)} \\
&\leq F_1 A_{d-1} C_d e^{\alpha_d |j|} \frac{\Gamma\left(|m|+|j|+\frac{d}{2}-1\right)}{\left(1-\frac{4\tau}{\omega_0}\right)^{|m|+|j|+\frac{d}{2}-1}} \sum_{k=0}^{\left[\!\left[\frac{|j|}{2}\right]\!\right]} \frac{e^{-2\alpha_d k}}{k!\Gamma\left(|j|-k+\frac{d}{2}\right)} \qquad (51)
\end{aligned}
$$

For $|j|\geq 1$, $|j|-k+d/2\geq 1+d/2\geq 2$ for all $0\leq k\leq \left[\!\left[\frac{|j|}{2}\right]\!\right]$. Since $\Gamma(x)$ is increasing for $x\geq 2$, we have

$$
\sum_{k=0}^{\left[\!\left[\frac{|j|}{2}\right]\!\right]} \frac{e^{-2\alpha_d k}}{k!\Gamma\left(|j|-k-\frac{d}{2}\right)} \leq \sum_{k=0}^{\left[\!\left[\frac{|j|}{2}\right]\!\right]} \frac{1}{k!(|j|-k)!} \leq \frac{1}{|j|!}\sum_{k=0}^{|j|} \begin{pmatrix} |j| \\ k \end{pmatrix} = \frac{1}{|j|!}2^{|j|}
$$

For $|j|=0$, the sum above is smaller than $2/\sqrt{\pi}$. Therefore

$$
\sum_{k=0}^{\left[\!\left[\frac{|j|}{2}\right]\!\right]} \frac{e^{-2\alpha_d k}}{k!\Gamma\left(|j|-k-\frac{d}{2}\right)} \leq \frac{2}{\sqrt{\pi}|j|!}2^{|j|}
$$

for all $|j|\geq 0$. Thus (51) becomes

$$
\left\| \frac{\delta^{|m|}}{m!} D^m V(\zeta) x^{m'} \left(1-\chi_R\right) \Phi_j(x) \right\|^2 \leq F_2 2^{|j|} e^{\alpha_d |j|} \frac{\Gamma\left(|m|+|j|+\frac{d}{2}-1\right)}{|j|!\left(1-\frac{4\tau}{\omega_0}\right)^{|m|+|j|+\frac{d}{2}-1}}
$$

with $F_2 := 2F_1 A_{d-1} C_d \pi^{-\frac{1}{2}}$.

Now consider any $\varphi\in \mathrm{Ran}\left(P_{|j|\leq 3n+a+1}\right)$ so $\varphi = \sum_{|j|\leq 3n+a+1} d_j \Phi_j(x)$. Then the Hölder inequality implies that

$$
\left\| \frac{\delta^{|m|}}{m!} D^m V(\zeta) x^{m'} \left(1-\chi_R\right) P_{|j|\leq a+3n+1}\varphi \right\|^2 \leq \|\varphi\|^2 \sum_{|j|\leq 3n+a+1} \left\| \frac{\delta^{|m|}}{m!} D^m V(\zeta) x^{m'} \left(1-\chi_R\right) \Phi_j(x) \right\|^2
$$

Therefore

$$
\left\| \frac{\delta^{|m|}}{m!} D^m V(\zeta) x^{m'} \left(1-\chi_R\right) P_{|j|\leq a+3n+1} \right\|^2
$$

$$
\begin{aligned}
&\le F_2 \frac{2^{3n+a+1} e^{\alpha_d(3n+a+1)}}{\left(1-\frac{4\tau}{\omega_0}\right)^{3n+|m|+a+\frac{d}{2}}} \sum_{|j|\le 3n+a+1} \frac{\Gamma\left(|m|+|j|+\frac{d}{2}-1\right)}{|j|!} \\
&\le F_2 \frac{2^{3n+a+1} e^{\alpha_d(3n+a+1)}}{\left(1-\frac{4\tau}{\omega_0}\right)^{3n+|m|+a+\frac{d}{2}}} \sum_{|j|\le 3n+a+1} \frac{(|m|+|j|+[\![d/2]\!]-1)!}{|j|!}
\end{aligned}
$$

where we use that $0<(1-4\tau/\omega_0)<1$. The terms under the summation sign are increasing in $|j|$. Also,

$$
\begin{aligned}
\sum_{|j|\le 3n+a+1} 1 &= \sum_{s=0}^{3n+a+1} \#\{j : |j|=s\} \\
&= \sum_{s=0}^{3n+a+1} \frac{(s+d-1)!}{s!(d-1)!} \\
&\le \sum_{s=0}^{3n+a+1} \frac{(s+d-1)^{d-1}}{(d-1)!} \\
&\le \frac{(3n+a+d)^{d-1}}{(d-1)!}(3n+a+2)
\end{aligned}
$$

Finally, $(3n+2+a)/(3n+1+a)\le 2$. Thus,

$$
\begin{aligned}
&\left\| \frac{\delta^{|m|}}{m!} D^m V(\zeta) x^{m'} \left(1-\chi_R\right) P_{|j|\le a+3n+1} \right\|^2 \\
&\qquad \le F_2 \frac{2^{3n+a+2} e^{\alpha_d(3n+a+1)}}{\left(1-\frac{4\tau}{\omega_0}\right)^{3n+|m|+a+\frac{d}{2}}} (3n+a+d)^{d-1} \frac{(3n+|m|+[\![d/2]\!]+a)!}{(3n+a)!}
\end{aligned}
$$

Finally, define F and G in the obvious way. $\square$

Theorem 3 *Given a, there are positive constants A , B and N_0 so that*

$$
\left\| A_e^{-1} \xi_N(x) \right\| \le \sum_{n=N}^{2N} A B^N \hbar^{\frac{N}{2}} [(2+a+n)!]^{\frac{1}{2}}
$$

whenever $N\ge N_0$ and $\hbar\le 1$.

Proof. Recall that we assume that $\delta\le 1$. We already know that $b\ge 1$. From the proof of Lemma 2, we also know that $\|x_\alpha A_e\|\le\gamma_1$.

From (47) it follows that

$$
\left\| A_e^{-1} \xi_N(x) \right\| \le \hbar^{\frac{N}{2}} \sum_{n=0}^{N-1} \sum_{|m|=N-n+2} \left\| \frac{D^m V\left(\zeta_n\right)}{m!} (1-\chi_R(x)) x^m A_e \psi_n(x) \right\|
$$

$$
\begin{aligned}
& + \hbar^{\frac{N}{2}} \sum_{n=0}^{N-1} \sum_{|m|=N-n+2} \left\| \frac{D^m V\left(\zeta_n\right)}{m!} \chi_R(x) x^m A_e \psi_n(x) \right\| \\
& + \sum_{n=N}^{2N-2} \hbar^{\frac{n}{2}} \sum_{l=n-N+1}^{N-1} \| \mathcal{E}_l A_e \psi_{n-l}(x) \| \\
\leq \; & \hbar^{\frac{N}{2}} \sum_{n=0}^{N-1} \sum_{|m|=N-n+2} \left\| \frac{D^m V\left(\zeta_n\right)}{m!} (1-\chi_R(x)) x^{m'} P_{|j| \leq 3n+a+1} \right\| \|x_\alpha A_e\| \, \|\psi_n(x)\| \\
& + \hbar^{\frac{N}{2}} \sum_{n=0}^{N-1} \sum_{|m|=N-n+2} \left\| \frac{D^m V\left(\zeta_n\right)}{m!} \chi_R(x) x^{m'} P_{|j| \leq 3n+a+1} \right\| \|x_\alpha A_e\| \, \|\psi_n(x)\| \\
& + \sum_{n=N}^{2N-2} \hbar^{\frac{n}{2}} \sum_{l=n-N+1}^{N-1} |\mathcal{E}_l| \, \|\psi_{n-l}(x)\|
\end{aligned}
$$

Let us estimates each term individually. Applying Lemma 4 and the estimates for $\|x_\alpha A_e\|$ and $\|\psi_n\|$, we obtain

$$
\begin{aligned}
1^{\text{st}} \text{ term} \;\; \leq \;\; & \hbar^{\frac{N}{2}} \sum_{n=0}^{N-1} \sum_{|m|=N+2-n} \delta^{|m|} F G^{\frac{3n+a+2}{2}} \left(1-\frac{4\tau}{\omega_0}\right)^{-\frac{|m|}{2}} (3n+a+d)^{\frac{d-1}{2}} \\
& \times \left[\frac{(3n+|m|+[\![d/2]\!]+a)!}{(3n+a)!} \right]^{\frac{1}{2}} \gamma_1 \kappa^{3n} b^{n+w} [(1+a+n)!]^{\frac{1}{2}} \\
\leq \;\; & F \gamma_1 \delta^{-(N+2)} G^{\frac{3N+a+d+1}{2}} \left(1-\frac{4\tau}{\omega_0}\right)^{-\frac{N+2}{2}} (3N+a+d-3)^{\frac{d-1}{2}} \\
& \times \sum_{n=0}^{N-1} \kappa^{3n} \left[\frac{(2n+N+[\![d/2]\!]+a+2)!(n+a+1)!}{(3n+a)!} \right]^{\frac{1}{2}} \sum_{|m|=N+2-n} 1
\end{aligned}
$$

Note that $(2n+N+[\![d/2]\!]+a+2)! \leq (2n+N+a+2)!(2n+N+[\![d/2]\!]+a+2)^{[\![d/2]\!]}$. Then

$$
\begin{aligned}
1^{\text{st}} \text{ term} \;\; \leq \;\; & A_1 B_1^N \hbar^{\frac{N}{2}} (3N+a+d-3)^{\frac{d-1}{2}} (N+d+1)^{d-1} (3N+a+[\![d/2]\!])^{\frac{[\![d/2]\!]}{2}} \\
& \times [(2+a+N)!]^{\frac{1}{2}} \sum_{n=0}^{N-1} \kappa^{3n} \left[\frac{(2+a+N+2n)!(1+a+n)!}{(a+3n)!(2+a+N)!} \right]^{\frac{1}{2}} \\
\leq \;\; & A_1 B_1^N \kappa^{3N} \hbar^{\frac{N}{2}} (3N+a+d-3)^{\frac{d-1}{2}} (N+d+1)^{d-1} (3N+a+[\![d/2]\!])^{\frac{[\![d/2]\!]}{2}} \\
& \times [(2+a+N)!]^{\frac{1}{2}} \max_{1 \leq l \leq N} \left[\frac{(3N-3l+a+1)(3N-3l+a+2)}{(N-l+a+2)} \right]^{\frac{1}{2}} \\
& \times \sum_{l=1}^{N} \kappa^{-\frac{5l}{2}} \left[\frac{(2+a+3N+2l)!(2+a+N-l)!}{(2+a+3N-3l)!(2+a+N)!} \right]^{\frac{1}{2}}
\end{aligned}
$$

where we use that $\sum_{|m|=N+2-n} 1 \leq [(d-1)!]^{-1}(N+d+1)^{d-1}$, and then we collect constants in A_1 and B_1. A change of index is performed in the summation above. Now we need to apply Lemma 3 to obtain

$$\begin{aligned} 1^{\text{st}} \text{ term} &\leq \beta A_1 B_1^N \kappa^{3N} \hbar^{\frac{N}{2}} (3N+a+d-3)^{\frac{d-1}{2}} (N+d+1)^{d-1} (3N+a+[\![d/2]\!])^{\frac{[\![d/2]\!]}{2}} \\ & \quad \times [3(3N+a+2)]^{\frac{1}{2}} [(2+a+N)!]^{\frac{1}{2}} \end{aligned}$$

Finally define N_1 through the inequality

$$(3N+a+[\![d/2]\!])^{\frac{[\![d/2]\!]}{2}} (3N_1+a+d-3)^{\frac{d-1}{2}} (N_1+d+1)^{d-1} [3(3N_1+a+2)]^{\frac{1}{2}} \leq \kappa^{N_1}$$

Then

$$1^{\text{st}} \text{ term} \leq \beta A_1 B_1^N \kappa^{4N} \hbar^{\frac{N}{2}} [(2+a+N)!]^{\frac{1}{2}}$$

whenever $N \geq N_1$.

Inequality (48) yields

$$\frac{\delta^{|m|}}{m!} |D^m V(\zeta(x))| \leq K \exp\left(\frac{2\tau d}{\omega_0^2} R^2\right) = K \exp\left[\frac{2\tau d}{\omega_0^2}(2a+d-4)\right] \exp\left(\frac{12\tau d}{\omega_0^2} N\right)$$

on the support of $\chi_R(x)$. Thus, the second term satisfies

$$\begin{aligned} 2^{\text{nd}} \text{ term} &\leq \hbar^{\frac{N}{2}} \gamma_1 \delta^{-(N+2)} K \exp\left[\frac{2\tau d}{\omega_0^2}(2a+d-4)\right] \exp\left(\frac{12\tau d}{\omega_0^2} N\right) \\ & \quad \times \sum_{n=0}^{N-1} \sum_{|m|=N-n+2} \left\| x^{m'} P_{|j| \leq 3n+a+1} \right\| \|\psi_n(x)\| \\ &\leq \hbar^{\frac{N}{2}} \gamma_1 \delta^{-(N+2)} K \exp\left[\frac{2\tau d}{\omega_0^2}(2a+d-4)\right] \exp\left(\frac{12\tau d}{\omega_0^2} N\right) \\ & \quad \times \sum_{n=0}^{N-1} \sum_{|m|=N-n+2} \kappa^{\frac{|m|-1}{2}} \left[\frac{(a+|m|+3n)!}{(1+a+3n)!}\right]^{\frac{1}{2}} \kappa^{3n} b^{n+w} [(1+a+n)!]^{\frac{1}{2}} \\ &\leq A_2 B_2^N \hbar^{\frac{N}{2}} (N+d+1)^{d-1} \sum_{n=0}^{N-1} \kappa^{3n} \left[\frac{(2+a+N+2n)!(1+a+n)!}{(1+a+3n)!}\right]^{\frac{1}{2}} \\ &\leq A_2 B_2^N \kappa^{3N} \hbar^{\frac{N}{2}} (N+d+1)^{d-1} [(2+a+N)!]^{\frac{1}{2}} \\ & \quad \times \max_{1 \leq l \leq N} \left[\frac{2+a+3N-3l}{2+a+N-l}\right]^{\frac{1}{2}} \sum_{l=1}^{N} \kappa^{-\frac{5l}{2}} \left[\frac{(2+a+3N+2l)!(2+a+N-l)!}{(2+a+3N-3l)!(2+a+N)!}\right]^{\frac{1}{2}} \\ &\leq 3^{\frac{1}{2}} \beta A_2 B_2^N \kappa^{3N} \hbar^{\frac{N}{2}} (N+d+1)^{d-1} [(2+a+N)!]^{\frac{1}{2}} \end{aligned}$$

Now define N_2 to satifies $(N_2+d+1)^{d-1} \leq \kappa^{N_2}$. Then for $N \geq N_2$

$$2^{\text{nd}} \text{ term} \leq 3^{\frac{1}{2}} \beta A_2 B_2^N \kappa^{4N} \hbar^{\frac{N}{2}} [(2+a+N)!]^{\frac{1}{2}}$$

For the third term we only need to use Lemma 1. The result is

$$3^{\text{rd}} \text{ term} \leq \sum_{n=N}^{2N} \gamma_a \kappa^{3n} b^{n+2w} \hbar^{\frac{N}{2}} [(1+a+n)!]^{\frac{1}{2}}$$

To complete the proof define $N_0 = \max\{N_1, N_2\}$, $A = \max\{\beta A_1, 3^{\frac{1}{2}}\beta A_2, \gamma_a b^{2w}\}$ and $B = \max\{\kappa^4 B_1, \kappa^3 B_2, \kappa^3 b\}$. □

5 Optimal truncation

In this section we prove that exact eigenvalues and eigenfunctions of $H(\hbar) := -\frac{1}{2}\Delta_x + V(\hbar, x)$ can be approximated by truncated R-S series, up to an exponentially small error. To that end, we will exploit our estimate of the norm $A_e^{-1}\xi_N(x)$. We will also need a couple of results. The first is a lower bound for the distance between perturbed eigenvalues that degenerate at $\hbar = 0$. The second is a "reverse" definition of asymptoticness, which is a generalization of Lemma 4 of [15].

Let us consider two distinct eigenvalues of $H(\hbar)$, $E(\hbar)$ and $E'(\hbar)$, which converge to the same eigenvalue of H_0 as $\hbar$ goes to 0. Also, let us assume that their asymptotic series have only a finite number of common R-S coefficients. That is,

$$\begin{aligned} E(\hbar) &\sim e + \mathcal{E}_1 \hbar^{\frac{1}{2}} + \ldots + \mathcal{E}_{M-1}\hbar^{\frac{M-1}{2}} + \mathcal{E}_M \hbar^{\frac{M}{2}} + \mathcal{E}_{M+1}\hbar^{\frac{M+1}{2}} + \ldots \\ E'(\hbar) &\sim e + \mathcal{E}_1 \hbar^{\frac{1}{2}} + \ldots + \mathcal{E}_{M-1}\hbar^{\frac{M-1}{2}} + \mathcal{E}'_M \hbar^{\frac{M}{2}} + \mathcal{E}'_{M+1}\hbar^{\frac{M+1}{2}} + \ldots \end{aligned}$$

with $\mathcal{E}_M \neq \mathcal{E}'_M$. Then,

$$E(\hbar) - E'(\hbar) \sim (\mathcal{E}_M - \mathcal{E}'_M)\, \hbar^{\frac{M}{2}} + \left(\mathcal{E}_{M+1} - \mathcal{E}'_{M+1}\right) \hbar^{\frac{M+1}{2}} + \ldots$$

so we expect that the difference between these exact eigenvalues be bounded below by $O\left(\hbar^{M/2}\right)$. Since the series above is asymptotic, there are $C_M > 0$ and $\hbar_1(M) > 0$ so that

$$\left| E(\hbar) - E'(\hbar) - (\mathcal{E}_M - \mathcal{E}'_M)\, \hbar^{\frac{M}{2}} \right| \leq C_M \hbar^{\frac{M+1}{2}}$$

whenever $\hbar \leq \hbar_1(M)$. Then

$$|E(\hbar) - E'(\hbar)| \geq |\mathcal{E}_M - \mathcal{E}'_M|\, \hbar^{\frac{M}{2}} - C_M \hbar^{\frac{M+1}{2}}$$

Set $\hbar_2(M) = |\mathcal{E}_M - \mathcal{E}'_M| / 2C_M$. Then for $\hbar \leq \hbar_2(M)$,

$$C_M \hbar^{\frac{M+1}{2}} \leq \frac{1}{2} |\mathcal{E}_M - \mathcal{E}'_M|\, \hbar^{\frac{M}{2}}$$

Thus for $\hbar \leq \min\{\hbar_1(M), \hbar_2(M)\}$ we have

$$|E(\hbar) - E'(\hbar)| \geq \frac{1}{2} |\mathcal{E}_M - \mathcal{E}'_M|\, \hbar^{\frac{M}{2}}$$

Let us denote $\mathcal{E}_M - \mathcal{E}'_M$ as $\Delta\mathcal{E}_M$. Therefore, so far we know that

Lemma 5 *Let $E(\hbar)$ and $E'(\hbar)$ be distinct eigenvalues of $H(\hbar)$, which degenerate at $\hbar = 0$. Then either*

1. $|E(\hbar) - E'(\hbar)| \leq O\left(\hbar^{\frac{N}{2}}\right)$ *for all non-negative integers N, or*

2. *There exist M and $\hbar_1 = \hbar_1(M)$ such that*

$$|E(\hbar) - E'(\hbar)| \geq \frac{1}{2}\,|\Delta\mathcal{E}_M|\,\hbar^{\frac{M}{2}}$$

whenever $\hbar \leq \hbar_1$.

Obviously this lemma is valid for several eigenvalues of $H(\hbar)$ converging to the same eigenvalue of H_0. As a shorthand, we will say that $E(\hbar)$ is *quasi-degenerate* if the condition 1 in the lemma above occurs.

Lemma 6 *Suppose $\sum_{n=0} f_n \beta^n$ is asymptotic to $f(\beta)$ in the sense that given $N \geq N_0 \geq M$, there exists C_N and $\beta(N)$ such that for all $\beta \leq \beta(N)$*

$$\left| f(\beta) - \sum_{n=0}^{N-1} f_n\,\beta^n \right| \;<\; C_N\,\beta^N.$$

Then given $\epsilon > 0$, there exists $\beta(\epsilon) > 0$, such that for each $\beta \leq \beta(\epsilon)$, there is an $N(\beta) \geq N_0$ (maybe equal to ∞), so that

$$\left| f(\beta) - \sum_{n=0}^{N-1} f_n\,\beta^n \right| \;\leq\; \epsilon\beta^M \tag{52}$$

whenever $N_0 \leq N < N(\beta)$.

Proof. Fix $\epsilon > 0$. Define $\beta_1(N_0) = (\epsilon\, C_{N_0}^{-1})^{\frac{1}{N_0-M}}$. Then for $N > N_0$, recursively choose positive numbers $\beta_1(N)$ that satisfy $\beta_1(N) < \min\{(\epsilon\, C_N^{-1})^{\frac{1}{N-M}},\, \beta_1(N-1)\}$. Then

$$\left| f(\beta) - \sum_{n=0}^{N-1} f_n\,\beta^n \right| \leq \left(C_N \beta^{N-M}\right)\beta^M \leq \left(C_N \beta_1(N)^{N-M}\right)\beta^M \leq \epsilon\beta^M$$

whenever $\beta < \beta_1(N)$.

Define $\beta(\epsilon) = \beta_1(N_0)$, and define

$$N(\beta) \;=\; \begin{cases} N+1 & \text{if} \quad \beta_1(N+1) < \beta \leq \beta_1(N) \\ \infty & \text{if} \quad \beta < \beta_1(N) \text{ for all } N. \end{cases}$$

Then (52) holds whenever $N_0 \leq N \leq N(\beta)$. $\square$

Let $\{e_\beta\}$ be an arrangement in increasing order of the eigenvalues of H_0, counting multiplicities. Theorem 1.1 of [14] states that given a non-negative integer α, we can choose $\hbar_0$ so that for each $\hbar \leq \hbar_0$ there are at least $\alpha + 1$ eigenvalues of $H(\hbar)$, counting multiplicities. Furthermore, each one of them converges to one of the first $\alpha + 1$ eigenvalues of H_0.

In the following proposition, we study the behavior of truncations of the R-S series of $E_\alpha(\hbar)$, the α-th eigenvalue of $H(\hbar)$. Without loss we may assume that $e_{\alpha+1} > e_\alpha$.

Proposition 3 *Let $E(\hbar) = E_\alpha(\hbar)$ be a non-quasi-degenerate eigenvalue of $H(\hbar)$, which converges to $e = e_\alpha$. Let $E_N(\hbar)$ be the associated R-S series, truncated at order N. Let N_0 be as defined in Theorem 3. Then there exists $\hbar_e > 0$ and so that for each $\hbar \leq \hbar_e$ there is an $N_e(\hbar) \geq N_0$ such that*

$$|E_N(\hbar) - E(\hbar)| \leq \sum_{n=N}^{2N} AB^n \hbar^{\frac{n}{2}} [(2 + a + n)!]^{\frac{1}{2}}$$

for all $\hbar \leq \hbar_e$ and $N_0 \leq N \leq N_e(\hbar)$.

Proof. If no other eigenvalue of $H(\hbar)$ converges to e, then the proof reduces to the one given in Proposition 3 of [15]. Otherwise, let $E'(\hbar)$ be another eigenvalue of $H(\hbar)$ converging to e as $\hbar \searrow 0$. By Lemma 5, there are M and $\hbar_1$ so that $|E(\hbar) - E'(\hbar)| \geq \frac{1}{2} |\Delta\mathcal{E}_M| \hbar^{\frac{M}{2}}$ for $\hbar \leq \hbar_1$. Without loss we may assume that $N_0 \geq M$. To simplify the proof, we furthermore assume that no other eigenvalue of $H(\hbar)$ converges to e.

Now set $N_1(\hbar)$ as the largest $N \geq N_0$ such that

$$\sum_{n=N_1(\hbar)}^{2N_1(\hbar)} AB^n \hbar^{\frac{n-M}{2}} [(2 + a + n)!]^{\frac{1}{2}} \leq \frac{1}{4} |\Delta\mathcal{E}_M|$$

Then, from Theorem 3 it follows that

$$\| [H(\hbar) - E_N(\hbar)]\, A_e \Psi_N(\hbar; x) \| \leq \sum_{n=N}^{2N} AB^n \hbar^{\frac{n}{2}} [(2 + a + n)!]^{\frac{1}{2}} \leq \frac{1}{4} |\Delta\mathcal{E}_M| \, \hbar^{\frac{M}{2}} \tag{53}$$

whenever $\hbar \leq \hbar_0$ (assumed to be less or equal than 1) and $N_0 \leq N \leq N_1(\hbar)$. By the same argument used in the proof of Proposition 3 of [15], the inequality above implies that

$$\operatorname{dist}\{E_N(\hbar), \sigma(H)\} \leq \sum_{n=N}^{2N} AB^n \hbar^{\frac{n}{2}} [(2 + a + n)!]^{\frac{1}{2}} \leq \frac{1}{4} |\Delta\mathcal{E}_M| \, \hbar^{\frac{M}{2}} \tag{54}$$

for $\hbar \leq \hbar_0$ and $N_0 \leq N \leq N_1(\hbar)$. Let Δ be minimum distance between distinct eigenvalues of H_0, among the first α+1 of them. Since $E_\beta(\hbar) \to e_\beta$, we can set $\hbar_\Delta > 0$ so that for $0 \leq \beta \leq \alpha$+1, $|E_\beta(\hbar) - e_\beta| \leq \frac{1}{4}\Delta$ if $\hbar \leq \hbar_\Delta$. That implies that, for $\hbar \leq \hbar_\Delta$ and $E''(\hbar) \in \sigma(H) \setminus \{E(\hbar), E'(\hbar)\}$,

$$\left| E^{\#}(\hbar) - E''(\hbar) \right| \geq \frac{1}{2}\Delta$$

where $E^{\#}$ denotes either E or E'. Now set $\hbar_2 = (\Delta / |\Delta\mathcal{E}_M|)^{\frac{2}{M}}$. Then for $\hbar \leq \hbar_2$ we have $\frac{1}{2}\Delta \geq \frac{1}{2} |\Delta\mathcal{E}_M| \hbar^{\frac{M}{2}}$. As a consequence,

$$\begin{aligned} |E(\hbar) - E''(\hbar)| &\geq \frac{1}{2} |\Delta\mathcal{E}_M| \hbar^{\frac{M}{2}} \\ |E(\hbar) - E'(\hbar)| &\geq \frac{1}{2} |\Delta\mathcal{E}_M| \hbar^{\frac{M}{2}} \end{aligned}$$

which ultimately implies that

$$\operatorname{dist}\{E(\hbar), \sigma(H) \setminus E(\hbar)\} \geq \frac{1}{2} |\Delta\mathcal{E}_M| \hbar^{\frac{M}{2}} \tag{55}$$

whenever $\hbar \leq \min\{\hbar_0, \hbar_1, \hbar_\Delta, \hbar_2\}$

Since $E_N(\hbar)$ is asymptotic to $E(\hbar)$, we may apply Lemma 6. Then there is $\hbar_3 > 0$ such that for each $\hbar \leq \hbar_3$ we can fix $N_2(\hbar) \geq N_0$ so that

$$|E(\hbar) - E_N(\hbar)| \leq \frac{1}{4} |\Delta\mathcal{E}_M| \hbar^{\frac{M}{2}} \tag{56}$$

for $N_0 \leq N \leq N_2(\hbar)$.

Now (55), (56) and the second inequality of (54) implies that

$$\operatorname{dist}\{E_N(\hbar), \sigma(H)\} = |E(\hbar) - E_N(\hbar)|$$

for $\hbar \leq \hbar_e = \min\{\hbar_0, \hbar_1, \hbar_\Delta, \hbar_2, \hbar_3\}$ and $N_0 \leq N \leq N_e(\hbar) \leq \min\{N_1(\hbar), N_2(\hbar)\}$. □

Remarks. The number $N_e(\hbar)$ defined in the proof must indeed be equal to $N_1(\hbar)$. For assume that $N_3(\hbar) < N_1(\hbar)$, and consider $N_3(\hbar) \leq N \leq N_1(\hbar)$. Then $E_N(\hbar)$ has to be near some eigenvalue $E''(\hbar)$ different to $E(\hbar)$. By reducing $\hbar$, $E_N(\hbar)$ approaches to $E(\hbar)$ but keeping itself close to $E''(\hbar)$, which leads to a contradiction. We must point out that this argument should be considered instead the one given in [15].

If $E(\hbar)$ is quasi-degenerate, then Proposition 3 is valid in the following weaker version:

Proposition 4 *Let $E(\hbar) = E_\alpha(\hbar)$ be an eigenvalue of $H(\hbar)$, which converges to $e = e_\alpha$. Let $E_N(\hbar)$ be the associated R-S series, truncated at order N. Also let $E^{\#}(\hbar)$ be any eigenvalue of $H(\hbar)$ that satisfies the condition 1 of Lemma 5 (including $E(\hbar)$ itself.) Then there exists $\hbar_e > 0$ so that for each $\hbar \leq \hbar_e$ there is an $N_e(\hbar) \geq N_0$ such that*

$$\left|E_N(\hbar) - E^{\#}(\hbar)\right| \leq \sum_{n=N}^{2N} AB^n \hbar^{\frac{n}{2}} [(2 + a + n)!]^{\frac{1}{2}}$$

for all $\hbar \leq \hbar_e$, $N_0 \leq N \leq N_e(\hbar)$, and $E^{\#}(\hbar)$.

In the following theorem we assume the hypotheses of Proposition 3. An analogous result follows from the hypotheses Proposition 4.

Theorem 4 *Assume the hypotheses of Proposition 3. Then for each* $0 < g < B^{-2}$*, there is* $\hbar_g > 0$ *such that for each* $\hbar \le \hbar_g$ *there exists* $N(\hbar)$ *such that*

$$\left|E_{N(\hbar)}(\hbar) - E(\hbar)\right| \le \Lambda \exp\left(-\frac{\Gamma}{\hbar}\right)$$

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

Proof. We follow the proof of Theorem 2 of [15]. So we only sketch the argument, pointing out the small changes needed here.

Fix $0 < g < B^{-2}$. Then we have $B^2 g = \exp(-\omega)$ for some $\omega > 0$. Consider the function

$$f(\hbar) := Ag \exp\left(-\frac{\omega(2+a)}{4}\right) \hbar^{-\frac{4+a+M}{2}} \exp\left(-\frac{\omega g}{4\hbar}\right)$$

and set

$$\hbar_4 = \inf\left\{\hbar : f(\hbar) \ge \frac{1}{4}\left|\Delta\mathcal{E}_M\right|\right\}$$

then set

$$\hat{\hbar}_g = \sup\left\{\hbar : \hbar \le \min\{\hbar_e, \hbar_4\} \text{ and } \left[\!\left[\frac{g}{\hbar}\right]\!\right] \ge 2 + a + 2N_0\right\}$$

Now for $\hbar \le \hat{\hbar}_g$ define $N(\hbar)$ by $2 + a + 2N(\hbar) = [\![\frac{g}{\hbar}]\!]$. So defined, $N(\hbar) \ge N_0$. Making a computation similar to one in the proof of Theorem 2 of [15], we can show that

$$\begin{aligned} \sum_{n=N(\hbar)}^{2N(\hbar)} AB^n \hbar^{\frac{n}{2}} \left[(2+a+n)!\right]^{\frac{1}{2}} &\le Age^{-\frac{\omega}{4}(1+a)} \hbar^{-\frac{4+a}{2}} \exp\left(-\frac{\omega g}{4\hbar}\right) \\ &\le \frac{1}{4}\left|\Delta\mathcal{E}_M\right| \hbar^{\frac{M}{2}} \end{aligned} \tag{57}$$

which means that $N(\hbar) \le N_e(\hbar)$. Thus, we can apply Proposition 3. Finally define

$$\hbar_g = \max\left\{\hbar \le \hat{\hbar}_g : \hbar^{-\frac{4+a}{2}} \exp\left(-\frac{\omega g}{8\hbar}\right) \le 1\right\}$$

Then, for each $\hbar \le \hbar_g$, Proposition 3 along with (57) implies the assertion. □

Similar results can be proven for eigenvectors, but only for non-quasi-degenerate eigenvalues of $H(\hbar)$. Recall that Ψ is an eigenvector of $H_e(\hbar)$ if and only if $\tilde{\Psi}$ is an eigenvector of $H(\hbar)$.

Proposition 5 *Let* $E(\hbar)$ *be a non-quasi-degenerate eigenvalue of* $H(\hbar)$*, with eigenspace* B_E*. Let* P_E *be the (orthogonal) projector onto* B_E*. Let* $\tilde{\Psi}_N(\hbar; x)$ *be the* N^{th} *truncation of the R-S series (6). Let* $\hbar_e$ *and* $N_e(\hbar)$ *be defined as in Proposition 3. Then for each* $\hbar \le \hbar_e$ *and* $N_0 \le N \le N_e(\hbar)$*,*

$$\left\| \frac{\tilde{\Psi}_N(\hbar; x)}{\left\|\tilde{\Psi}_N(\hbar; x)\right\|} - \frac{P_E \tilde{\Psi}_N(\hbar; x)}{\left\|P_E \tilde{\Psi}_N(\hbar; x)\right\|} \right\| \le 8\left|\Delta\mathcal{E}_M\right|^{-1} \sum_{n=N}^{2N} AB^n \hbar^{n-M} [(2+a+n)!]^{\frac{1}{2}}$$

for some $M \le N_0$.

Proof. As before, we only need to make a couple of changes to the proof of Proposition 3 of [15]. So details of the following argument can be found there.

We have

$$\left\|\tilde{\Psi}_N(\hbar;x)\right\|^{-1}\tilde{\Psi}_N(\hbar;x)=w_N\left\|P_E\tilde{\Psi}_N(\hbar;x)\right\|^{-1}P_E\tilde{\Psi}_N(\hbar;x)+\Omega_N(\hbar;x)$$

where $\Omega_N(\hbar;x)$ is orthogonal to B_E, and $|w_N|^2+\|\Omega_N(\hbar;x)\|^2=1$. Then we can prove that

$$\left\|\left\|\tilde{\Psi}_N(\hbar;x)\right\|^{-1}\tilde{\Psi}_N(\hbar;x)-\left\|P_E\tilde{\Psi}_N(\hbar;x)\right\|^{-1}P_E\tilde{\Psi}_N(\hbar;x)\right\|\leq 2\left\|\Omega_N(\hbar;x)\right\| \tag{58}$$

On the other hand, (53) implies that

$$\left\|[H(\hbar)-E_N(\hbar)]\left\|\tilde{\Psi}_N(\hbar;x)\right\|^{-1}\tilde{\Psi}_N(\hbar;x)\right\|\leq\sum_{n=N}^{2N}AB^n\hbar^{\frac{n}{2}}[(2+a+n)!]^{\frac{1}{2}}$$

from which, after some algebra, Proposition 3 implies that

$$\left\|[H(\hbar)-E_N(\hbar)]\,\Omega_N(\hbar;x)\right\|\leq 2\sum_{n=N}^{2N}AB^n\hbar^{\frac{n}{2}}[(2+a+n)!]^{\frac{1}{2}} \tag{59}$$

for $\hbar\leq\hbar_e$ and $N_0\leq N\leq N_e(\hbar)$.

Recall that $E_N(\hbar)\notin\sigma(H)$. From the fact that $[H(\hbar)-E_N(\hbar)]\,\Omega_N(\hbar;x)$ is orthogonal to B_E, it follows that

$$\left\|\Omega_N(\hbar;x)\right\|\leq\left\|[H(\hbar)-E_N(\hbar)]_\perp^{-1}\right\|\left\|[H(\hbar)-E_N(\hbar)]\,\Omega_N(\hbar;x)\right\| \tag{60}$$

where $[H(\hbar)-E_N(\hbar)]_\perp$ is the restriction of $[H(\hbar)-E_N(\hbar)]$ to the subspace orthogonal to B_E. For simplicity, let us assume that $E'(\hbar)$ converges to the same eigenvalue of H_0 as $E(\hbar)$. Then (55) and the spectral theorem imply that

$$\left\|[H(\hbar)-E_N(\hbar)]_\perp^{-1}\right\|\leq\left(\operatorname{dist}\left\{E(\hbar),\sigma(H)\setminus E(\hbar)\right\}\right)^{-1}\leq 2\left|\Delta\mathcal{E}_M\right|^{-1}\hbar^{-\frac{M}{2}} \tag{61}$$

Now the assertion follows from (58)–(61). □

Remarks. The assumption of non-quasi-degeneracy of $E(\hbar)$ is critical, as one can see in the argument that leads (61).

The optimal truncation for eigenvectors follows from Proposition 5 as Theorem 4 does from Proposition 3:

Theorem 5 *For $0\leq g\leq B^{-2}$ there is Λ', Γ' and $\hbar'_g>0$ such that for each $\hbar\leq\hbar_g$ there is $N'(\hbar)$ so that*

$$\left\|\frac{\tilde{\Psi}_{N(\hbar)}(\hbar;x)}{\left\|\tilde{\Psi}_{N(\hbar)}(\hbar;x)\right\|}-\frac{P_E\tilde{\Psi}_{N(\hbar)}(\hbar;x)}{\left\|P_E\tilde{\Psi}_{N(\hbar)}(\hbar;x)\right\|}\right\|\leq\Lambda'\exp\left(-\frac{\Gamma'}{\hbar}\right)$$

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6 Appendix

Here we simplify the formula (46) by using the identity (10). This calculation is formally identical the one done in [15], with some notational change. We reproduce it here for a sake of convenience.

$$\begin{aligned}\xi_N &= \left[H_e + A_e W A_e - \sum_{j=1}^{N-1} \hbar^{\frac{j}{2}} \mathcal{E}_j A_e^2\right] \sum_{m=0}^{N-1} \hbar^{\frac{m}{2}} \psi_m \\ &= \sum_{m=0}^{N-1} \hbar^{\frac{m}{2}} H_e \psi_m + \sum_{m=0}^{N-1} \hbar^{\frac{m}{2}} A_e W A_e \psi_m - \sum_{j=1}^{N-1} \sum_{m=0}^{N-1} \hbar^{\frac{j+m}{2}} \mathcal{E}_j A_e^2 \psi_m\end{aligned}$$

We use $A_e W A_e = \sum_{j=3}^{N+2} \hbar^{\frac{j-2}{2}} T^{(j)} + A_e W^{[N+2]} A_e$ and change the index by $j \to j-2$. Using $H_e \psi_0 = 0$, we then obtain

$$\begin{aligned}\xi_N &= \sum_{m=1}^{N-1} \hbar^{\frac{m}{2}} H_e \psi_m + \sum_{m=0}^{N-1} \sum_{j=1}^{N} \hbar^{\frac{m+j}{2}} T^{(j+2)} \psi_m \\ &\quad + \sum_{m=0}^{N-1} \hbar^{\frac{m}{2}} A_e W^{[N+2]} A_e \psi_m - \sum_{m=0}^{N-1} \sum_{j=1}^{N-1} \hbar^{\frac{j+m}{2}} \mathcal{E}_j A_e^2 \psi_m \\ &= \sum_{n=1}^{N-1} \hbar^{\frac{n}{2}} H_e \psi_n + \sum_{n=1}^{N-1} \hbar^{\frac{n}{2}} \sum_{j=1}^{n} T^{(j+2)} \psi_{n-j} \\ &\quad + \sum_{n=N}^{2N-1} \hbar^{\frac{n}{2}} \sum_{j=n-N+1}^{N} T^{(j+2)} \psi_{n-j} + \sum_{m=0}^{N-1} \hbar^{\frac{m}{2}} A_e W^{[N+2]} A_e \psi_m \\ &\quad - \sum_{n=1}^{N-1} \hbar^{\frac{n}{2}} \sum_{j=1}^{n} \mathcal{E}_j A_e^2 \psi_{n-j} - \sum_{n=N}^{2N-2} \hbar^{\frac{n}{2}} \sum_{j=n-N+1}^{N-1} \mathcal{E}_j A_e^2 \psi_{n-j}\end{aligned}$$

The first, second and fifth terms of last equation cancel because of (10). In the third term define $m = n - j$ and then $p = n - N$. This yields

$$\begin{aligned}\xi_N &= \sum_{n=N}^{2N-1} \hbar^{\frac{n}{2}} \sum_{m=n-N}^{N-1} T^{(n-m+2)} \psi_m \\ &\quad + \sum_{m=0}^{N-1} \hbar^{\frac{m}{2}} A_e W^{[N+2]} A_e \psi_m - \sum_{n=N}^{2N-2} \hbar^{\frac{n}{2}} \sum_{j=n-N+1}^{N-1} \mathcal{E}_j A_e^2 \psi_{n-j} \\ &= \sum_{p=0}^{N-1} \sum_{m=p}^{N-1} \hbar^{\frac{p+N}{2}} T^{(p+N-m+2)} \psi_m \\ &\quad + \sum_{m=0}^{N-1} \hbar^{\frac{m}{2}} A_e W^{[N+2]} A_e \psi_m - \sum_{n=N}^{2N-2} \hbar^{\frac{n}{2}} \sum_{j=n-N+1}^{N-1} \mathcal{E}_j A_e^2 \psi_{n-j}\end{aligned}$$

$$
\begin{aligned}
&= \sum_{m=0}^{N-1} \hbar^{\frac{m}{2}} \sum_{p=0}^{m} \hbar^{\frac{p+N-m}{2}} T^{(p+N-m+2)} \psi_m \\
&\quad + \sum_{m=0}^{N-1} \hbar^{\frac{m}{2}} A_e W^{[N+2]} A_e \psi_m - \sum_{n=N}^{2N-2} \hbar^{\frac{n}{2}} \sum_{j=n-N+1}^{N-1} \mathcal{E}_j A_e^2 \psi_{n-j} \\
&= \sum_{m=0}^{N-1} \hbar^{\frac{m}{2}} \left[\sum_{i=2}^{m+2} \hbar^{\frac{i+N-m-2}{2}} T^{(i+N-m)} + A_e W^{[N+2]} A_e \right] \psi_m \\
&\quad - \sum_{n=N}^{2N-2} \hbar^{\frac{n}{2}} \sum_{j=n-N+1}^{N-1} \mathcal{E}_j A_e^2 \psi_{n-j}
\end{aligned}
$$

Finally, note that $\hbar^{\frac{j-2}{2}} T^{(j)} + A_e W^{[j+1]} A_e = A_e W^{[j]} A_e$. It then follows that

$$
\xi_N = \sum_{m=0}^{N-1} \hbar^{\frac{m}{2}} A_e W^{[N-m+1]} A_e \psi_m - \sum_{n=N}^{2N-2} \hbar^{\frac{n}{2}} \sum_{j=n-N+1}^{N-1} \mathcal{E}_j A_e^2 \psi_{m-j}
$$

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