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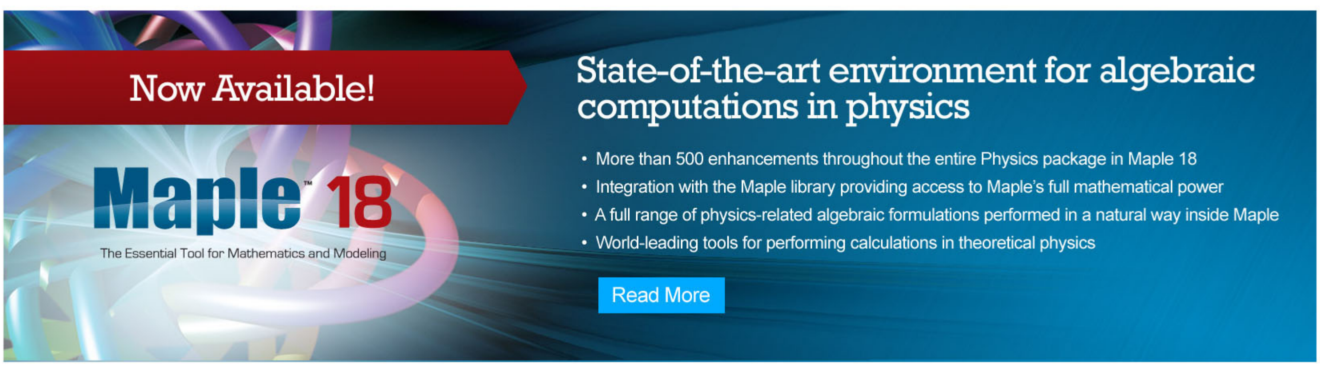

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Exponentially accurate error estimates of quasiclassical eigenvalues. II. Several dimensions

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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 the one-dimensional case in a previous article. This time we consider the multi-dimensional problem, where degeneracy plays a central role. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1581353]

I. INTRODUCTION

Perhaps one of the most elementary facts in quantum physics is that, for a sufficiently deep potential well, the eigenvalue problem defined by the time-independent Schrödinger equation admits normalizable solutions. Equivalently, if one considers Planck's constant as a parameter, the equation

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

is expected to have eigenvalues near the bottom of the potential well, in the semiclassical limit $\hbar\searrow 0$.

Along with the problem of existence of low-lying eigenvalues, one is also interested in the behavior of the corresponding perturbation series in powers of $\hbar$, the so-called Rayleigh–Schrödinger (R-S) series. It is well known that, in general, the R-S series are not convergent but only asymptotic to the solutions of Eq. (1). However, one often wants to consider truncations of these series as good approximations to the actual eigenvalues/eigenvectors. This raises the natural question of whether or not one can find an optimal truncation that minimizes the difference between the exact eigenvalues/eigenvectors and the corresponding truncated R-S series.

In this article we aim to find exponentially accurate asymptotics to the solutions of (1). We shall assume that the potential energy $V(x)$ satisfies the following conditions:

H1 $V(x)$ is a C^∞ real function on $\mathbb{R}^d$ such that $\liminf_{|x|\to\infty}V(x)=:V_\infty>0$.

H2 $V(x)$ has a unique global minimum $V(0)=0$ at $x=0$.

H3 The global minimum of $V(x)$ is nondegenerate in the sense that

$$\mathrm{Hess}_V(0)=\mathrm{diag}[\omega_1^2,\ldots,\omega_d^2]$$

has only strictly positive eigenfrequencies $\omega_1,\ldots,\omega_d$.

H4 $V(x)$ has an analytic extension to a neighborhood of the region $S_\delta=\{z:|\mathrm{Im}\, z_i|\leqslant\delta+\epsilon\}$ for some

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$\delta>0$ and $\epsilon>0$ arbitrarily small. Without loss we may assume that $\delta\leqslant 1$.

H5 $V(z)$ satisfies $|V(z)|\leqslant M\exp(\tau|z|^2)$ uniformly in S_δ, for some positive constants $M>0$ and $\omega_0/4\geqslant\tau>0$ where ω_0 denotes the lowest eigenfrequency of $\mathrm{Hess}_V(0)$.

We shall prove that one can truncate the R-S series so that the difference between the truncated series and the actual eigenvalue/eigenvector can be made smaller than $\Lambda\exp(-\Gamma/\hbar)$ where the positive constants Λ and Γ are explicitly calculated. Our construction is based entirely on a straighforward application of the formal R-S perturbation theory. These results extend those in Ref. 19, where we discussed optimal truncation for the one-dimensional problem. We follow the method explained in that article, which indeed is related with one developed by Hagedorn and Joye to study approximate solutions to the time-dependent Schrödinger equation.[4] 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 $ab^N\hbar^{N/2}(N!)^{1/2}$. 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 Ref. 19 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.

The study of this problem is not new, of course. The first proof of existence of low-lying eigenvalues and asymptotic R-S series was presented by Combes *et al.* in 1983. Their proof, which involves Dirichlet–Newmann bracketing techniques, only considers the one-dimensional problem. Shortly after, Simon gave another proof, based on geometric arguments, that is valid in several dimensions.[16] This problem was also studied by Helffer and Sjöstrand in the broader framework of microlocal analysis of self-adjoint pseudodifferential operators.[6] From these works, it is known that eigenvalues/eigenfunctions near the bottom of the potential well admit asymptotic expansions in half-powers of $\hbar$, where the leading orders are given by the corresponding eigenvalues/eigenfunctions of the harmonic oscillator aproximation. These results require only to assume that the potential energy satisfies H1–H3, although further information has been obtained in Ref. 6 for potentials with analytic continuation in a neighborhood of the minimum. In particular, it is proved in Theorem 4.6 of Ref. 6 that the low-lying eigenvalues/eigenfunctions can be exponentially approximated by truncated series.

The last result mentioned above is based on the rather involved theory of analytic pseudodifferential operators.[18] On the other hand, the work by Hagedorn and Joye[4] suggests that a much simpler method, involving only formal R-S series, may be used to contruct exponentially accurate aproximations to the eigenvalues/eigenfunctions of (1). Indeed, the constructive method developed in this work relies upon only some elementary notions on complex and functional analysis. Moreover, we obtain explicit upper bounds to the growth of the R-S coefficients. Our construction might be used for numerical computation, although the many constants that we define along the way have not been optimized for that purpose. However, there is a tradeoff in our approach which consists on the need of somewhat stronger assumptions about the potential energy, namely, hypothesis H5. We finally would like to point out that our technique could be used to study the time-independent Born–Oppenheimer approximation.

Results analogous to those discussed in this work have also been obtained for a class of C^∞ potentials. Bambusi *et al.*[1] have studied exponentially accurate quasimodes up to an error of order $\exp(-\mathrm{const}/\hbar^{1/\rho})$ with $\rho>1$, when the potential energy is Gevrey of order $\mu>1$. Furthermore, their estimate on the error is uniform in $\hbar$ for all eigenvalues in $[0,\hbar^\delta]$ with $0<\delta<1$. The construction of those quasimodes is based upon quantization of the Birkhorff normal forms for the classical Hamiltonian associated to (1). Since their proof relies on the KAM theorem,[3] the authors assume that the eigenfrequencies $\omega_1,\dots,\omega_d$ satisfy the nonresonant condition $|\Sigma_i\omega_i k_i|^{-1}\leqslant C(\Sigma_i|k_i|)^\alpha$, for $C>0$, $\alpha>0$, and for every nontrivial set of integers $(k_1,\dots,k_d)$. Under similar assumptions, Popov[12,13] has proved more general results by quantization of the KAM theory.

This article is organized as follows. In Sec. II we make a transformation of Eq. (1), and some technical results are proven. In Sec. III we construct some operators through recursion relations,

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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 Sec. II, we obtain a manageable recursion relation for the nth term of the R-S series. Then we state and prove an estimate of the growth of these terms. In Sec. IV we define a residual error function for Eq. (1) and prove an estimate for it. The main results are stated precisely in Sec. V. The Appendix is devoted to a computation needed in Sec. IV.

II. PRELIMINARIES

In this work we shall use the standard multi-index notation: for $\alpha=(\alpha_1,\ldots,\alpha_d)\in\mathbb{Z}_+^d$ and $x=(x_1,\ldots,x_d)\in\mathbb{R}^d$, we denote $|\alpha|:=\alpha_1+\cdots+\alpha_d$, $\alpha!:=\alpha_1!\cdot\cdots\cdot\alpha_d!$, $x^\alpha:=x_1^{\alpha_1}\cdot\cdots\cdot x_d^{\alpha_d}$, $D^\alpha:=\partial_{x_1}^{\alpha_1}\cdot\cdots\cdot\partial_{x_d}^{\alpha_d}$, and $x^2:=x_1^2+\cdots+x_d^2$. For $z=(z_1,\ldots,z_d)\in\mathbb{C}^d$, we denote $|z|^2:=z_1z_1^*+\cdots+z_dz_d^*$.

We first transform (1) by scaling $x\to\hbar^{1/2}x$ and then dividing the whole equation by $\hbar$. This unitary transformation scales the eigenvalues and eigenfunctions as $E\to\hbar^{-1}E$ and $\tilde{\Psi}(x)\to\tilde{\Psi}(\sqrt{\hbar}x)$, respectively. The transformed equation may be written as

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

Because of hypothesis H3, $V(x)$ admits a Taylor expansion up to any order n. Thus we can write

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

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

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

Hypothesis H4 implies furthermore that the Taylor series (3) is convergent inside the open polydisc $\{z\in\mathbb{C}^d:|z_i|\leqslant\delta\}$. Upper bounds on the derivatives of $V(x)$ can be easily obtained by using the Cauchy integral formula. They are stated and proved below in Lemma 2.

Now we can rewrite (2) as

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

where, in suitable Cartesian coordinates,

$$H_0=-\frac{1}{2}\Delta_x+\frac{1}{2}\sum_{i=1}^{d}\omega_i^2x_i^2$$

is a harmonic oscillator Hamiltonian with eigenfrequencies $\omega_1,\ldots,\omega_d$. The eigenfunctions of H_0 are therefore

$$\Phi_\alpha(x)=\left(\pi^{-d}\prod_{i=1}^{d}\omega_i\right)^{1/4}(2^{|\alpha|}\alpha!)^{-1/2}\exp\left(-\frac{1}{2}\sum_{i=1}^{d}\omega_ix_i^2\right)\prod_{i=1}^{d}h_{\alpha_i}(\sqrt{\omega_i}x_i), \tag{5}$$

where $h_j(y)$ denotes the Hermite polynomial of degree j. The corresponding eigenvalues are $e_\alpha=\Sigma_{i=1}^{d}\omega_i\alpha_i+d/2$.

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

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

$$E(\hbar) \sim \mathcal{E}_0 + \hbar^{1/2}\mathcal{E}_1 + \hbar^{2/2}\mathcal{E}_2 + \hbar^{3/2}\mathcal{E}_3 + \hbar^{4/2}\mathcal{E}_4 + \cdots. \tag{7}$$

In this work we essentially follow the standard, formal method to compute the R-S coefficients (see, e.g., Ref. 11, Chap. XVI), although alternatively we could use the technique developed by Kato (Ref. 10 Chaps. VII and VIII). 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.[8,9]

We now insert (6) and (7) into (2) and equate powers of $\hbar^{1/2}$. The zeroth-order equation yields $H_0\psi_0 = \mathcal{E}_0\psi_0$. Then $\mathcal{E}_0 = e$ and $\psi_0 \in G$, where e is some eigenvalue of H_0 with multiplicity g and associated eigenspace G. For $n=1,2,\ldots,$ we have

$$(H_0 - e)\tilde{\psi}_n + \sum_{l=1}^{n} \tilde{T}^{(l+2)}\tilde{\psi}_{n-l} = \sum_{l=1}^{n} \mathcal{E}_l\tilde{\psi}_{n-l}, \tag{8}$$

where we define

$$\tilde{T}^{(l)} := \sum_{|\alpha|=l} \frac{1}{\alpha!} D^{\alpha}V(0)x^{\alpha}.$$

Existence of solutions to the set of equations (8) can be shown by explicit construction, as the one we shall develop in Sec. III. Also, the correction terms $\tilde{\psi}_n$ satisfies the following property:

Lemma 1: Let $P_{|\alpha|\leq l}$ *be the projection onto the subspace spanned by* $\{\Phi_\alpha : |\alpha| \leq l\}$ *and* $a = a_e$ *be the smallest non-negative integer such that* $G \subseteq \mathrm{Ran}(P_{|\alpha|\leq a})$. *Then, for each* $n \geq 1$, $\tilde{\psi}_n \in \mathrm{Ran}(P_{|\alpha|\leq a+3n})$

Proof: First, decompose $\tilde{\psi}_n = P_{|\alpha|\leq a}\tilde{\psi}_n + (1 - P_{|\alpha|\leq a})\tilde{\psi}_n =: \tilde{\psi}_n^{(1)} + \tilde{\psi}_n^{(2)}$. We have to prove the assertion only for $\tilde{\psi}_n^{(2)}$. Equation (8) yields

$$\tilde{\psi}_n^{(2)} = (H_0 - e)_r^{-1}(1 - P_{|\alpha|\leq a})\left[\sum_{l=1}^{n} \mathcal{E}_l\tilde{\psi}_{n-l} - \sum_{l=1}^{n} \tilde{T}^{(l+2)}\tilde{\psi}_{n-l}\right],$$

where $(H_0 - e)_r^{-1}$ is the inverse of the restriction of $H_0 - e$ onto $\mathrm{Ran}(1 - P_{|\alpha|\leq a})$. Since

$$\mathrm{Ran}((H_0 - e)_r^{-1}(1 - P_{|\alpha|\leq a})P_{|\alpha|\leq a+3n}) \subset \mathrm{Ran}(P_{|\alpha|\leq a+3n}),$$

it is sufficient to show that

$$\left(\sum_{l=1}^{n} \mathcal{E}_l\tilde{\psi}_{n-l} - \sum_{l=1}^{n} \tilde{T}^{(l+2)}\tilde{\psi}_{n-l}\right) \in P_{|\alpha|\leq a+3n}. \tag{9}$$

Now use mathematical induction. For $n=1$, the assertion $\tilde{T}^{(3)}\tilde{\psi}_0 \in P_{|\alpha|\leq a+3}$ follows from the fact that $\tilde{T}^{(3)}$ contains terms that are at most proportional to the third power of creation operators, and that $\tilde{\psi}_0 \in G \subset P_{|\alpha|\leq a}$. Assuming that statement is true for $s=1,\ldots,n-1$, then it is trivially true for the first term in (9). Also, a simple calculation with ladder operators shows that $x^{\alpha}\varphi \in \mathrm{Ran}(P_{|\beta|\leq a+3(n-l)+|\alpha|})$ whenever $\varphi \in \mathrm{Ran}(P_{|\beta|\leq a+3(n-l)})$. Finally, we have $3(n-l)+2+l = 3n + 2(1-l) \leq 3n$ for $l=1,\ldots,n$. □

The set of recursive equations (8) is not suitable for the purpose of finding the sharp upper bounds for the R-S coefficients that we shall need later. It turns out to be convenient to transform the problem in the following way: Let $\{\Phi_\alpha(x)\}$ be a basis of eigenvectors of H_0. For a given eigenvalue e of H_0, let us define a new operator A_e by

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$$A_e\Phi_\alpha(x) = \begin{cases} \Phi_\alpha(x), & \text{if } \Phi_\alpha(x)\in G, \\ |e-e_\alpha|^{-1/2}\Phi_\alpha(x), & \text{otherwise,} \end{cases}$$

where e_α is the eigenvalue associated to $\Phi_\alpha(x)$. Then extend A_e to the whole Hilbert space $\mathcal{H}$ by linearity. So defined, A_e is a bounded operator with unit norm but unbounded inverse. However, $\mathrm{Ran}(P_{|\alpha|\leqslant a+3n})$ is clearly in the domain of A_e^{-1} for each $n\in\mathbb{N}$. This fact allows us to consider the equivalent set of equations

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

where $H_e := A_e(H_0-e)A_e$, $T^{(m)} := A_e\tilde{T}^{(m)}A_e$, and $\psi_m = A_e^{-1}\tilde{\psi}_m$. The operator H_e satisfies

$$H_e\Phi_\alpha(x) = \begin{cases} 0, & \text{if } \Phi_\alpha(x)\in G, \\ \dfrac{e-e_\alpha}{|e-e_\alpha|}\Phi_\alpha(x), & \text{otherwise.} \end{cases}$$

Therefore the norm of H_e is equal to 1. In Sec. III we shall prove that both $|\mathcal{E}_n|$ and $\|\psi_n\|$ essentially grow as $b^n\sqrt{n!}$ for large n.

We conclude this section with an assortment of technical lemmas. Lemma 2 states certain estimates on the derivatives of the potential energy. In Lemma 3 we show a key upper bound to the norm of the operators $T^{(l)}P_{|\alpha|\leqslant n}$. Finally, in Lemma 4 we state results about certain expressions involving factorials that we shall use extensively in the sequel.

Lemma 2: Assume $V(x)$ satisfies H4. Then there are constants C_1 and C_2 such that, for $l \geqslant 1$,

$$\sum_{|\alpha|=l} \frac{|D^\alpha V(0)|}{\alpha!}\delta^{|\alpha|} \leqslant C_1 C_2^l.$$

If $V(x)$ also satisfies H5, then there exists a constant C_0 such that

$$\frac{\delta^{|\alpha|}}{\alpha!}|D^\alpha V(x)| \leqslant C_0 \exp(2\tau x^2). \tag{11}$$

Proof: Let Γ_i be a circle of radius δ in the complex plane, centered at x_i. Then the Cauchy integral formula applied to $V(x)$, which makes sense because of hypothesis H4, states that for each multi-index $\alpha=(\alpha_1,\dots,\alpha_d)$

$$D^\alpha V(x) = \frac{\alpha!}{(2\pi i)^d}\int_{\Gamma_1} dz_1 \cdots \int_{\Gamma_d} dz_d \frac{V(z)}{\prod_{i=1}^d (z_i-x_i)^{\alpha_i+1}},$$

which implies

$$|D^\alpha V(x)| \leqslant \frac{\alpha!}{\delta^{|\alpha|}} \max_{z_i\in\Gamma_i}|V(z)|. \tag{12}$$

Let us prove (11) first. Because of H5,

$$\max_{z_i\in\Gamma_i}|V(z)| \leqslant M\prod_{i=1}^{d} \max_{z_i\in\Gamma_i}\exp(\tau|z_i|^2) \leqslant M\prod_{i=1}^{d} \exp(\tau|x_i+\delta|^2) \leqslant M\exp(2d\tau\delta^2)\exp(2\tau x^2),$$

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so (12) implies (11), after defining $C_0 = M \exp(2d\tau\delta^2)$. If now the Γ_i's are circles centered at zero, we have (without assuming H5)

$$\frac{|D^\alpha V(0)|}{\alpha!}\delta^{|\alpha|} \leqslant \max_{z_i \in \Gamma_i} |V(z)| =: c < \infty.$$

Then

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

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,

$$\sum_{|\alpha|=l} 1 = \frac{(l+d-1)!}{l!(d-1)!} \leqslant \frac{1}{(d-1)!}(l+d-1)^{d-1}.$$

Therefore, we have

$$\sum_{|\alpha|=l} \frac{|D^\alpha V(0)|}{\alpha!}\delta^{|\alpha|} \leqslant \frac{c}{(d-1)!}(l+d-1)^{d-1} \leqslant C_1 C_2^l$$

with obvious definition of C_1, and C_2 being either equal to $(d-1)\max_{l\geqslant 1}\log(l+d-1)/l$ (when $d>1$) or equal to 1 (when $d=1$). □

Lemma 3: For $|\alpha| \geqslant 2$, $n \geqslant 0$ *and some constant* $\gamma > 0$,

$$\|A_e x^\alpha A_e P_{|\beta|\leqslant n}\| \leqslant \gamma^2 \left(\frac{2}{\omega_0}\right)^{(|\alpha|-2)/2} \left[\frac{(n+|\alpha|-1)!}{(n+1)!}\right]^{1/2}.$$

As a consequence,

$$\|T^{(l)} P_{|\beta|\leqslant n}\| \leqslant C_3 \kappa^{(l-2)/2} \left[\frac{(n+l-1)!}{(n+1)!}\right]^{1/2}$$

for some $C_3 > 0$ *and* $\kappa \geqslant 2$.

Proof: For a single coordinate x_i, we have

$$x_i = \frac{1}{\sqrt{2\omega_i}}(a_i + a_i^*) \tag{13}$$

where a_i and a_i^* are the associated ladder operators. Consider any $\varphi = \Sigma_\beta d_\beta \Phi_\beta \in \mathcal{H}$. Define $J_G := \{\text{multi-indices } \beta : \Phi_\beta \in G\}$. Then

$$\begin{aligned} a_i^* A_e \varphi &= \sum_{\beta \in J_G} d_\beta a_i^* \Phi_\beta + \sum_{\beta \notin J_G} d_\beta |e - e_\beta|^{-1/2} a_i^* \Phi_\beta \\ &= \sum_{\beta \in J_G} d_\beta \sqrt{\beta_i + 1}\, \Phi_{\beta + 1_i} + \sum_{\beta \notin J_G} d_\beta |e - e_\beta|^{-1/2} \sqrt{\beta_i + 1}\, \Phi_{\beta + 1_i} \end{aligned}$$

where $\beta + 1_i := (\beta_1, \ldots, \beta_i + 1, \ldots, \beta_d)$. Thus,

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$$\|a_i^* A_e \varphi\|^2 = \sum_{\beta \in J_G} |d_\beta|^2 (\beta_i + 1) + \sum_{\beta \notin J_G} |d_\beta|^2 |e - e_\beta|^{-1} (\beta_i + 1)$$
$$\leq (1+a) \sum_{\beta \in J_G} |d_\beta|^2 + \sum_{\beta \notin J_G} |d_\beta|^2 |e - e_\beta|^{-1} (\beta_i + 1)$$

because $\beta \in J_G$ implies $\beta_i \leq |\beta| \leq a$. Moreover,

$$\frac{\beta_i + 1}{|e - e_\beta|} = \frac{1}{\omega_i} \frac{\omega_i(\beta_i + \frac{1}{2})}{|e - e_\beta|} + \frac{\frac{1}{2}}{|e - e_\beta|} \leq \frac{1}{\omega_i} \frac{e_\beta}{|e - e_\beta|} + \frac{\frac{1}{2}}{|e - e_\beta|}.$$

Since $\sigma(H_0)$ has no accumulation points and $e_\beta \neq e$ for all $\beta \notin J_G$, $\inf_{\beta \notin J_G} |e - e_\beta| > 0$. Furthermore, since $\lim_{|\beta| \to \infty} e_\beta |e - e_\beta|^{-1} = 1$, $\sup_{\beta \notin J_G} e_\beta |e - e_\beta|^{-1} < \infty$. Thus,

$$|e - e_\beta|^{-1} (\beta_i + 1) \leq \frac{1}{\omega_i} \sup_{\beta \notin J_G} e_\beta |e - e_\beta|^{-1} + \frac{1}{2} \sup_{\beta \notin J_G} |e - e_\beta|^{-1} =: K_1 < \infty,$$

which implies

$$\|a_i^* A_e\|^2 \leq \max\{(1+a), K_1\} \leq \max_{\{\omega_i\}} \max\{(1+a), K_1\}. \tag{14}$$

A similar calculation yields

$$\|a_i A_e\|^2 \leq \max\{|1-a|, K_2\} \leq \max_{\{\omega_i\}} \max\{|1-a|, K_2\} \tag{15}$$

for some $K_2 < \infty$. Therefore,

$$\|x_i A_e\| \leq \frac{1}{\sqrt{2\omega_i}} \|a_i A_e\| + \frac{1}{\sqrt{2\omega_i}} \|a_i^* A_e\| \leq \frac{1}{\sqrt{2\omega_0}} (\|a_i A_e\| + \|a_i^* A_e\|) \leq \gamma,$$

where ω_0 is the lowest eigenfrequency of H_0, and we use the sum of the right-hand sides of (14) and (15) to define γ. Taking the adjoint yields

$$\|A_e x_i\| \leq \gamma.$$

Since $|\alpha| \geq 2$, we can write $x^\alpha = x_i x^{\alpha'} x_j$ for some x_i, x_j, with $|\alpha'| = |\alpha| - 2$. Then

$$\|A_e x^\alpha A_e P_{|\beta| \leq n}\| \leq \|A_e x_i x^{\alpha'} P_{|\beta| \leq n+1} x_j A_e P_{|\beta| \leq n}\|$$
$$\leq \|A_e x_i\| \|x_j A_e\| \|x^{\alpha'} P_{|\beta| \leq n+1}\|$$
$$\leq \gamma^2 \left(\frac{2}{\omega_0}\right)^{|\alpha'|/2} \left[\frac{(n + |\alpha'| + 1)!}{(n+1)!}\right]^{1/2}$$
$$= \gamma^2 \left(\frac{2}{\omega_0}\right)^{(|\alpha|-2)/2} \left[\frac{(n + |\alpha| - 1)!}{(n+1)!}\right]^{1/2}, \tag{16}$$

where we use Lemma 5.1 of Ref. 4 to bound $\|x^{\alpha'} P_{|\beta| \leq n+1}\|$. The last statement follows from the definition of $T^{(l)}$ and the first part of Lemma 2, along with the definitions $C_3 = C_1 \gamma^2 \delta^{-2} C_2^2$ and $\kappa = \max\{2, 2\omega_0^{-1} \delta^{-2} C_2^2\}$. □

Lemma 4: Let $\kappa \geq 2$ be the number defined in Lemma 3. Then we have the following.

(1) For each integer $a \geq 0$ there is a constant $C_4 = C_4(a)$ so that, for all $m \geq 0$,

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$$\sum_{l=0}^{m}\left[\frac{(1+a+m-l)!(1+a+l)!}{(1+a+m)!}\right]^{1/2}\leqslant C_4 .$$

(2) For all $a\geqslant -1$ *there is a constant* C_5 *so that, for all* $m\geqslant 0$,

$$\sum_{l=0}^{m}\kappa^{-5l/2}\left[\frac{(1+a+3m-2l)!(1+a+m-l)!}{(1+a+3m-3l)!(1+a+m)!}\right]^{1/2}\leqslant C_5 .$$

(3) For each $a\geqslant 0$ *there is a constant* $C_6=C_6(a)$ *so that, for all* $m\geqslant 0$,

$$\sum_{l=1}^{m}\kappa^{-5l/2}\left[\frac{(1+a+m-l)!(1+a+l)!}{(1+a)!(a+m)!}\right]^{1/2}\leqslant C_6 .$$

Proof: Statements (1) and (2) are shown in Lemma 2 of Ref. 19. To prove (3), notice that for $1\leqslant l\leqslant m-1$ we have

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

Therefore

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

where the right-hand side converges to some constant $C_6(a)<\infty$. □

III. COMPUTATION OF THE R-S COEFFICIENTS

Let us assume that the zeroth-order eigenvalue e is g-fold degenerate, with associated eigenspace G. We allow g to be equal to 1. Let P be the projector onto G and $Q:=1-P$. Up to zeroth-order, ψ_0 can be any vector in G, 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 nondegenerate one.

A. Degeneracy is preserved

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

$$H_e\psi_1+T^{(3)}\psi_0=\mathcal{E}_1A_e^2\psi_0 . \tag{17}$$

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 secular equation 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 λ_1. Then $\mathcal{E}_1=\lambda_1$. Now multiply (17) by Q. We obtain

$$H_eQ\psi_1=-QT^{(3)}\psi_0 .$$

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

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

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

The second-order equation is

$$H_e\psi_2 + T^{(3)}\psi_1 + T^{(4)}\psi_0 = \mathcal{E}_2 A_e^2\psi_0 + \lambda_1 A_e^2\psi_1 . \tag{18}$$

Multiply (18) by P. After some algebra involving the definitions of $\Lambda^{(1)}$ and $\Xi^{(1,\perp)}$, we obtain

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

Then $\mathcal{E}_2$ has to be equal to the unique eigenvalue of

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

That is, $\mathcal{E}_2 = \lambda_2$. Now multiply (18) by Q to obtain

$$H_e\psi_2^\perp + QT^{(3)}(\psi_1^\parallel + \psi_1^\perp) + QT^{(4)}\psi_0 = \lambda_1 A_e^2\psi_1^\perp ,$$

which yields

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

where we define

$$\Xi^{(2,\perp)} := (H_e)_\perp^{-1}[(\lambda_1 A_e^2 - QT^{(3)})\Xi^{(1,\perp)} + QT^{(4)}]$$

and no requirement is imposed on either $\psi_2^\parallel$ or $\psi_1^\parallel$.

The third-order equation is

$$H_e\psi_3 + T^{(3)}\psi_2 + T^{(4)}\psi_1 + T^{(5)}\psi_0 = \mathcal{E}_3 A_e^2\psi_0 + \lambda_2 A_e^2\psi_1 + \lambda_1 A_e^2\psi_2 .$$

Following the procedure already described, we obtain

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

where

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

has only one eigenvalue λ_3. Thus $\mathcal{E}_3 = \lambda_3$. Also

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

where

$$\Xi^{(3,\perp)} := (H_e)_\perp^{-1}[(\lambda_1 A_e^2 - QT^{(3)})\Xi^{(2,\perp)} + (\lambda_2 A_e^2 - QT^{(4)})\Xi^{(1,\perp)} - QT^{(5)}]$$

and nothing is said about $\psi_3^\parallel$, $\psi_2^\parallel$ or $\psi_1^\parallel$.

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

$$\Xi^{(1,\perp)} := -(H_e)_\perp^{-1}QT^{(3)},$$

$$\Xi^{(n,\perp)} := (H_e)_\perp^{-1}\left[-QT^{(n+2)} + \sum_{p=1}^{n-1}(\lambda_{n-p}A_e^2 - QT^{(n+2-p)})\Xi^{(p,\perp)}\right],$$

where λ_l is, by assumption, the unique eigenvalue of

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

Then, given $\psi_0 \in G$, $\mathcal{E}_n = \lambda_n$ *and*

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

where $\psi_1^{\parallel},\dots,\psi_n^{\parallel}$ *are vectors arbitrarily chosen from* G.

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 $\psi_n^{\parallel}=0$ for all $n \geqslant 1$, which is equivalent to absorbing those vectors into ψ_0 and renormalizing.

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

$$\mathcal{E}_n = \sum_{p=0}^{n-1} \langle T^{(n+2-p)}P_{|\alpha|\leqslant a}\psi_0, \psi_p\rangle,$$

$$\psi_n = (H_e)_\perp^{-1}\left[-QT^{(n+2)}\psi_0 + \sum_{p=1}^{n-1} (\mathcal{E}_{n-p}A_e^2 - QT^{(n+2-p)})\psi_p \right].$$

Furthermore, we can easily obtain the following inequalities:

$$|\mathcal{E}_n| \leqslant \sum_{l=1}^{n} \|T^{(l+2)}P_{|j|\leqslant a}\| \|\psi_{n-l}\|,$$

$$\|\psi_n\| \leqslant \sum_{l=1}^{n-1} |\mathcal{E}_l| \|\psi_{n-l}\| + \sum_{l=1}^{n} \|T^{(l+2)}P_{|j|\leqslant a+3(n-l)}\| \|\psi_{n-l}\|.$$

By resorting to Lemma 3, we finally obtain

$$|\mathcal{E}_n| \leqslant C_3 \sum_{l=1}^{n} \kappa^{l/2}\left[\frac{(1+a+l)!}{(1+a)!}\right]^{1/2} \|\psi_{n-l}\|,$$

$$\|\psi_n\| \leqslant \sum_{l=1}^{n-1} |\mathcal{E}_l| \|\psi_{n-l}\| + C_3 \sum_{l=1}^{n} \kappa^{l/2}\left[\frac{(1+a+3n-2l)!}{(1+a+3n-3l)!}\right]^{1/2} \|\psi_{n-l}\|.$$

As an immediate consequence, we have the following.

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

$$|\mathcal{E}_n| \leqslant \kappa^{3n} b^n [(1+a+n)!]^{1/2},$$

$$\|\psi_n\| \leqslant \kappa^{3n} b^n [(1+a+n)!]^{1/2},$$

for all $n \geqslant 1$.

A proof of this theorem is in Ref. 19, where the somewhat simpler one-dimensional problem is discussed. Alternatively, one can modify the proof of Theorem 3.2 below to get somewhat tighter bounds.

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B. 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 $k\geqslant 2$ distinct eigenvalues $\lambda_{1,1},\ldots,\lambda_{1,k}$. Let $G_1,\ldots,G_k$ be the corresponding eigenspaces, and let $P^{(1)},\ldots,P^{(k)}$ be their orthogonal projections. Set $\mathcal{E}_1=\lambda_{1,i}$. Then ψ_0 must lie in G_i. As before, $\psi_1^{\perp}=\Xi^{(1,\perp)}\psi_0$ with $\Xi(1,\perp)$ $:=(He)\perp-1(-QT(3))$.

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

$$H_e\psi_2+T^{(3)}\psi_1+T^{(4)}\psi_0=\mathcal{E}_2A_e^2\psi_0+\lambda_{1,i}A_e^2\psi_1. \tag{19}$$

Multiply (19) by $P^{(j)}$

$$P^{(j)}T^{(3)}\psi_1+P^{(j)}T^{(4)}\psi_0=\mathcal{E}_2P^{(j)}\psi_0+\lambda_{1,i}P^{(j)}\psi_1. \tag{20}$$

Note that $P=\Sigma_{j=1}^{k}P^{(j)}$. Then, for any vector ψ, we have $\psi^{\parallel}=\Sigma_{j=1}^{k}\psi^{(j)}$. On the other hand,

$$P^{(j)}T^{(3)}\psi^{\parallel}=\sum_{l=1}^{k}P^{(j)}PT^{(3)}PP^{(l)}\psi^{\parallel}=\sum_{l=1}^{k}P^{(j)}\Lambda^{(1)}P^{(l)}\psi^{\parallel}=\sum_{l=1}^{k}\lambda_{1,l}P^{(j)}P^{(l)}\psi^{\parallel}=\lambda_{1,j}\psi^{(j)}. \tag{21}$$

Therefore, $\Sigma_{l\neq i}P^{(i)}T^{(3)}\psi_n^{(l)}=0$. The identity (21) yields

$$P^{(j)}T^{(3)}\psi_1=P^{(j)}T^{(3)}\psi_1^{\parallel}+P^{(j)}T^{(3)}\psi_1^{\perp}=\lambda_{1,j}\psi_1^{(j)}+P^{(j)}T^{(3)}\psi_1^{\perp}. \tag{22}$$

Now insert (22) into (20). For $j=i$ we have

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

Define

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

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

For $j\neq i$ we have

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

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

$$\Xi^{(1,j)}:=(\lambda_{1,i}-\lambda_{1,j})^{-1}P^{(j)}(T^{(4)}+T^{(3)}\Xi^{(1,\perp)})P^{(i)}. \tag{23}$$

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

Now multiply (19) by Q,

$$H_e\psi_2^{\perp}+QT^{(4)}\psi_0+QT^{(3)}\psi_1=\lambda_{1,i}A_e^2\psi_1^{\perp}. \tag{24}$$

Since

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

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(24) yields

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

From there we obtain

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

where

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

Third-order:

$$H_e\psi_3+T^{(3)}\psi_2+T^{(4)}\psi_1+T^{(5)}\psi_0=\mathcal{E}_3A_e^2\psi_0+\lambda_{2,i}A_e^2\psi_1+\lambda_{1,i}A_e^2\psi_2. \tag{25}$$

Multiply by $P^{(j)}$, rearrange terms, and use (21) to obtain

$$\begin{aligned}\mathcal{E}_3P^{(j)}\psi_0&=P^{(j)}T^{(3)}\psi_2+P^{(j)}T^{(4)}\psi_1+P^{(j)}T^{(5)}\psi_0-\lambda_{2,i}\psi_1^{(j)}-\lambda_{1,i}\psi_2^{(j)}\\&=P^{(j)}T^{(3)}(\psi_2^{\perp}+\psi_2^{\parallel})+P^{(j)}T^{(4)}\left(\psi_1^{\perp}+\sum_{l\neq i}\psi_1^{(l)}+\psi_1^{(i)}\right)\\&\quad+P^{(j)}T^{(5)}\psi_0-\lambda_{2,i}\psi_1^{(j)}-\lambda_{1,i}\psi_2^{(j)}\\&=P^{(j)}T^{(3)}\psi_2^{\perp}+P^{(j)}T^{(4)}\left(\psi_1^{\perp}+\sum_{l\neq i}\psi_1^{(i)}+\psi_1^{(i)}\right)\\&\quad+P^{(j)}T^{(5)}\psi_0-(\lambda_{1,i}-\lambda_{1,j})\psi_2^{(j)}-\lambda_{2,i}\psi_1^{(j)}.\end{aligned} \tag{26}$$

For $j=i$ we have

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

Let us note that

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

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 $\lambda_{3,i}$ so $\mathcal{E}_3=\lambda_{3,i}$.

Now for $j\neq i$ we can rewrite (26) as

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

Now use (23) and define

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

to obtain

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

The last step is to multiply (25) by Q,

$$H_e\psi_3^{\perp}=Q(\lambda_{1,i}A_e^2-T^{(3)})\psi_2+Q(\lambda_{2,i}A_e^2-T^{(4)})\psi_1-QT^{(5)}\psi_0. \tag{27}$$

We have

$$\begin{aligned}Q(\lambda_{1,i}A_e^2-T^{(3)})\psi_2&=Q(\lambda_{1,i}A_e^2-T^{(3)})\psi_2^{\perp}+\lambda_{1,i}A_e^2Q\psi_2^{\parallel}-QT^{(3)}\sum_{l\neq i}\psi_2^{(l)}-QT^{(3)}\psi_2^{(i)}\\&=Q(\lambda_{1,i}A_e^2-T^{(3)})\Xi^{(2,\perp)}\psi_0+Q(\lambda_{1,i}A_e^2-T^{(3)})\Xi^{(1,i)}\psi_1^{(i)}\\&\quad-QT^{(3)}\sum_{l\neq i}\Xi^{(2,l)}\psi_0-QT^{(3)}\sum_{l\neq i}\Xi^{(1,l)}\psi_1^{(i)}-QT^{(3)}\psi_2^{(i)}\\&=-QT^{(3)}\psi_2^{(i)}+Q\left[(\lambda_{1,i}A_e^2-T^{(3)})\Xi^{(1,\perp)}-\sum_{l\neq i}T^{(3)}\Xi^{(1,l)}\right]\psi_1^{(1)}\\&\quad+Q\left[(\lambda_{1,i}A_e^2-T^{(3)})\Xi^{(2,\perp)}-\sum_{l\neq i}T^{(3)}\Xi^{(2,l)}\right]\psi_0,\end{aligned} \tag{28}$$

and similarly

$$Q(\lambda_{2,i}A_e^2-T^{(4)})\psi_1=Q\left[(\lambda_{2,i}A_e^2-T^{(4)})\Xi^{(1,\perp)}-\sum_{l\neq i}T^{(4)}\Xi^{(1,l)}\right]\psi_0-QT^{(4)}\psi_1^{(i)}. \tag{29}$$

Insert (28) and (29) in (27) 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

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

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

Proposition 2: Define

$$\Lambda^{(1)}:=PT^{(3)}P,$$

$$\Xi^{(1,\perp)}:=-(H_e)_\perp^{-1}QT^{(3)}.$$

Suppose that $\Lambda^{(1)}$ has k distinct eigenvalues $\lambda_{1,1},\ldots,\lambda_{1,k}$ with eigenspaces $G_1,\ldots,G_k$. Let $P^{(1)},\ldots,P^{(k)}$ be the associated projection operators. Given $1\leqslant i\leqslant k$ and $j\neq i$, set

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

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$$\Xi^{(1,j)} := (\lambda_{1,i} - \lambda_{1,j})^{-1} P^{(j)} (T^{(4)} + T^{(3)} \Xi^{(1,\perp)}) P^{(i)},$$

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

And then recursively define

$$\Lambda^{(n,i)} := P^{(i)} \left(T^{(n+2)} + \sum_{s=1}^{n-1} T^{(n+2-s)} \Xi^{(s,\perp)} + \sum_{s=1}^{n-2} \sum_{l \neq i} T^{(n+2-s)} \Xi^{(s,l)} \right) P^{(i)},$$

$$\Xi^{(n-1,j)} := (\lambda_{1,i} - \lambda_{1,j})^{-1} P^{(j)} \left(T^{(n+2)} + \sum_{s=1}^{n-1} T^{(n+2-s)} \Xi^{(s,\perp)} + \sum_{s=1}^{n-2} \sum_{l \neq i} T^{(n+2-s)} \Xi^{(s,l)} - \sum_{s=2}^{n-1} \lambda_{s,i} \Xi^{(n-s,j)} \right) P^{(i)},$$

$$\Xi^{(n,\perp)} := (H_e)_\perp^{-1} \left[\sum_{s=1}^{n-1} \lambda_{s,i} \Xi^{(n-s,\perp)} A_e^2 - Q T^{(n+2)} - \sum_{s=1}^{n-1} Q T^{(s+2)} \left(\Xi^{(n-s,\perp)} + \sum_{l \neq i} \Xi^{(n-s,l)} \right) \right],$$

where $\lambda_{s,i}$ is, by assumption, the unique eigenvalue of $\Lambda^{(s,i)}$ when $s \geqslant 2$.

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 $\mathcal{E}_1 = \lambda_{1,i}$. Consequently, $\psi_0 \in G_i$ and

$$\mathcal{E}_n = \lambda_{n,i}, \tag{30}$$

$$\psi_{n-1}^{(j)} = \Xi^{(n-1,j)} \psi_0 + \sum_{s=1}^{n-1} \Xi^{(n-s-1,j)} \psi_s^{(i)}, \tag{31}$$

$$\psi_n^{\perp} = \Xi^{(n,\perp)} \psi_0 + \sum_{s=1}^{n-1} \Xi^{(n-s,\perp)} \psi_s^{(i)}, \tag{32}$$

$$\psi_n = \psi_n^{\perp} + \sum_{j \neq i} \psi_n^{(j)} + \psi_n^{(i)}.$$

The vectors $\psi_1^{(i)}, \dots, \psi_n^{(i)}$ are arbitrarily chosen from G_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 (30)–(32), for $m = 2, \dots, n$. Let us compute $\mathcal{E}_{n+1}$, $\psi_n^{(j)}$ and $\psi_{n+1}^{\perp}$. The $(n+1)$-st-order equation is

$$H_e \psi_{n+1} + \sum_{p=0}^{n} T^{(n+3-p)} \psi_p = \sum_{s=0}^{n} \mathcal{E}_{n+1-s} A_e^2 \psi_s. \tag{33}$$

We have

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$$\sum_{p=0}^{n} T^{(n+3-p)}\psi_p = T^{(n+3)}\psi_0 + \sum_{p=1}^{n} T^{(n+3-p)}\psi_p^{\perp} + \sum_{p=1}^{n} T^{(n+3-p)}\sum_{l\neq i}\psi_p^{(l)} + \sum_{p=1}^{n} T^{(n+3-p)}\psi_p^{(i)}$$

$$= T^{(n+3)}\psi_0 + T^{(n+2)}\Xi^{(1,\perp)}\psi_0 + \sum_{p=2}^{n} T^{(n+3-p)}\left(\Xi^{(p,\perp)}\psi_0 + \sum_{s=1}^{p-1}\Xi^{(p-s,\perp)}\psi_s^{(i)}\right)$$

$$+ d\sum_{l\neq i} T^{(n+2)}\Xi^{(1,l)}\psi_0 + \sum_{p=2}^{n-1}\sum_{l\neq i} T^{(n+3-p)}\left(\Xi^{(p,l)}\psi_0 + \sum_{s=1}^{p-1}\Xi^{(p-s,l)}\psi_s^{(i)}\right)$$

$$+ \sum_{l\neq i} T^{(3)}\psi_n^{(l)} + \sum_{p=1}^{n} T^{(n+3-p)}\psi_p^{(i)}$$

$$= \left(T^{(n+3)} + \sum_{p=1}^{n} T^{(n+3-p)}\Xi^{(p,\perp)} + \sum_{p=1}^{n-1}\sum_{l\neq i} T^{(n+3-p)}\Xi^{(p,l)}\right)\psi_0$$

$$+ \sum_{s=1}^{n-1}\sum_{p=s+1}^{n} T^{(n+3-p)}\Xi^{(p-s,\perp)}\psi_s^{(i)}$$

$$+ \sum_{s=1}^{n-2}\sum_{p=s+1}^{n-1}\sum_{l\neq i} T^{(n+3-p)}\Xi^{(p-s,l)}\psi_s^{(i)} + \sum_{l\neq i} T^{(3)}\psi_n^{(l)} + \sum_{s=1}^{n} T^{(n+3-s)}\psi_s^{(i)}$$

$$= \left(T^{(n+3)} + \sum_{p=1}^{n} T^{(n+3-p)}\Xi^{(p,\perp)} + \sum_{p=1}^{n-1}\sum_{l\neq i} T^{(n+3-p)}\Xi^{(p,l)}\right)\psi_0$$

$$+ \sum_{s=1}^{n-1}\sum_{m=1}^{n-s} T^{(n+3-s-m)}\Xi^{(m,\perp)}\psi_s^{(i)} + \sum_{s=1}^{n-2}\sum_{m=1}^{n-1-s}\sum_{l\neq i} T^{(n+3-s-m)}\Xi^{(m,l)}\psi_s^{(i)}$$

$$+ \sum_{l\neq i} T^{(3)}\psi_n^{(l)} + \sum_{s=1}^{n} T^{(n+3-s)}\psi_s^{(i)}$$

where we use that $\Sigma_{p=1}^{r}\Sigma_{s=1}^{p-1}F_{sp} = \Sigma_{s=1}^{r-1}\Sigma_{p=s+1}^{r}F_{sp}$ and then we change index $p\to m = p-s$. Let us multiply (33) by $P^{(i)}$. Since $P^{(i)}H_e = 0$ and $P^{(i)}A_e^2 = A_e^2 P^{(i)} = P^{(i)}$, we obtain

$$\sum_{p=0}^{n} P^{(i)}T^{(n+3-p)}\psi_p = \mathcal{E}_{n+1}\psi_0 + \sum_{s=1}^{n}\lambda_{n+1-s,i}\psi_s^{(i)}. \tag{34}$$

The left-hand side can be written as

$$\sum_{p=0}^{n} P^{(i)}T^{(n+3-p)}\psi_p = P^{(i)}\left(T^{(n+3)} + \sum_{p=1}^{n} T^{(n+3-p)}\Xi^{(p,\perp)} + \sum_{p=1}^{n-1}\sum_{l\neq i} T^{(n+3-p)}\Xi^{(p,l)}\right)\psi_0$$

$$+ \sum_{s=1}^{n-2} P^{(i)}\left(T^{(n+3-s)} + \sum_{m=1}^{n-s} T^{(n+3-s-m)}\Xi^{(m,\perp)}\right.$$

$$\left. + \sum_{m=1}^{n-1-s}\sum_{l\neq i} T^{(n+3-s-m)}\Xi^{(m,l)}\right)\psi_s^{(i)} + P^{(i)}(T^{(3)}\Xi^{(1,\perp)} + T^{(4)})\psi_{n-1}^{(i)}$$

$$+ \sum_{l\neq i} P^{(i)}T^{(3)}\psi_n^{(l)} + P^{(i)}T^{(3)}\psi_n^{(i)}.$$

By the argument that leads to (21), we know that $\Sigma_{l\neq i}P^{(i)}T^{(3)}\psi_n^{(l)} = 0$. Also $\psi_s^{(i)} = P^{(i)}\psi_s^{(i)}$. Then

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$$\sum_{p=0}^{n} P^{(i)}T^{(n+3-p)}\psi_p=\Lambda^{(n+1,i)}\psi_0+\sum_{s=1}^{n}\Lambda^{(n+1-s,i)}\psi_s^{(i)}. \tag{35}$$

Inserting (35) into (34) we conclude

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

Now let us multiply (33) by $P^{(j)}$ for $j\neq i$. Since $P^{(j)}\psi_0=0$, we have

$$\lambda_{1,i}\psi_n^{(j)}=\sum_{p=0}^{n} P^{(j)}T^{(n+3-p)}\psi_p-\sum_{s=1}^{n-1}\lambda_{n+1-s,i}\psi_s^{(j)}. \tag{36}$$

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

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

As proven in (21), the last term above is equal to $\lambda_{1,j}\psi_n^{(j)}$. Thus (36) leads to

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

Finally, multiply (33) by Q,

$$H_e\psi_{n+1}^{\perp}=\sum_{p=1}^{n}\lambda_{n+1-p,i}A_e^2\psi_p^{\perp}-\sum_{p=0}^{n}QT^{(n+3-p)}\psi_p. \tag{37}$$

For the first term we have

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

and for the second one

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

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Then insert these expressions into (37). After multiplying the whole equation by $(H_e)_\perp^{-1}$ we obtain the desired result. □

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:

$$\Lambda^{(n,i)}\psi_0=P^{(i)}T^{(n+2)}\psi_0+\sum_{s=1}^{n-2}P^{(i)}T^{(n+2-s)}\psi_s+P^{(i)}T^{(3)}\psi_{n-1}^{\perp},\tag{38}$$

$$\psi_n^{\perp}=(H_e)_\perp^{-1}\left[\sum_{s=1}^{n-1}\mathcal{E}_sA_e^2\psi_{n-s}^{\perp}-QT^{(n+2)}\psi_0-\sum_{s=1}^{n-1}QT^{(s+2)}\psi_{n-s}\right],\tag{39}$$

$$\psi_{n-1}^{(j)}=(\lambda_{1,i}-\lambda_{1,j})^{-1}\Bigg(P^{(j)}T^{(n+2)}\psi_0+\sum_{s=1}^{n-2}P^{(j)}T^{(n+2-s)}\psi_s+P^{(j)}T^{(3)}P_{|j|\leqslant a+3(n-1)}\psi_{n-1}^{\perp}$$
$$-\sum_{s=2}^{n-1}\mathcal{E}_s\psi_{n-s}^{(j)}\Bigg).\tag{40}$$

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

$$\begin{aligned}|\mathcal{E}_n|&=|\langle\psi_0,\Lambda^{(n,i)}\psi_0\rangle|\\
&\leqslant|\langle\psi_0,P^{(i)}T^{(n+2)}\psi_0\rangle|+\sum_{s=1}^{n-2}|\langle\psi_0,P^{(i)}T^{(n+2-s)}\psi_s\rangle|+|\langle\psi_0,P^{(i)}T^{(3)}\psi_{n-1}^{\perp}\rangle|\\
&\leqslant\|T^{(n+2)}P_{|\alpha|\leqslant a}\|+\sum_{s=1}^{n-2}|\langle T^{(n+2-s)}\psi_0,\psi_s\rangle|+|\langle T^{(3)}\psi_0,\psi_{n-1}^{\perp}\rangle|\\
&\leqslant\|T^{(n+2)}P_{|\alpha|\leqslant a}\|+\sum_{s=1}^{n-2}\|T^{(n+2-s)}P_{|\alpha|\leqslant a}\|\|\psi_s\|+\|T^{(3)}P_{|\alpha|\leqslant a}\|\|\psi_{n-1}^{\perp}\|\\
&=\sum_{s=2}^{n}\|T^{(s+2)}P_{|\alpha|\leqslant a}\|\|\psi_{n-s}\|+\|T^{(3)}P_{|\alpha|\leqslant a}\|\|\psi_{n-1}^{\perp}\|.\end{aligned}\tag{41}$$

This calculation follows from (38), the self-adjointness of $T^{(l)}$, and Lemma 1.

From the definition of H_e, it is straightforward to see that $\|(H_e)_\perp^{-1}\|=1$. Also, $\|A_e\|=1$. Thus, from (39) we have

$$\begin{aligned}\|\psi_n^{\perp}\|&\leqslant\sum_{s=1}^{n-1}|\mathcal{E}_s|\|\psi_{n-s}^{\perp}\|+\|T^{(n+2)}P_{|\alpha|\leqslant a}\|\|\psi_0\|+\sum_{s=1}^{n-1}\|T^{(s+2)}P_{|\alpha|\leqslant a+3(n-s)}\|\|\psi_{n-s}\|\\
&=\sum_{s=1}^{n-1}|\mathcal{E}_s|\|\psi_{n-s}^{\perp}\|+\sum_{s=1}^{n}\|T^{(s+2)}P_{|\alpha|\leqslant a+3(n-s)}\|\|\psi_{n-s}\|.\end{aligned}\tag{42}$$

Finally let us consider (40):

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$$\|\psi_{n-1}^{(j)}\| \leqslant |\lambda_{1,i}-\lambda_{1,j}|^{-1}\left(\|T^{(n+2)}P_{|\alpha|\leqslant a}\|\|\psi_0\| + \sum_{s=1}^{n-2} \|P^{(j)}T^{(n+2-s)}\|\|\psi_s\| + \|P^{(j)}T^{(3)}\|\|\psi_{n-1}^{\perp}\| + \sum_{s=2}^{n-1} |\mathcal{E}_s|\|\psi_{n-s}^{(j)}\| \right).$$

Set $C_7 := \min_{j\neq i}|\lambda_{1,i}-\lambda_{1,j}|^{-1}$. Also, let us notice that $\|P^{(j)}T^{(n+2-s)}\| = \|T^{(n+2-s)}P^{(j)}\| = \|T^{(n+2-s)}P_{|\alpha|\leqslant a}P^{(j)}\| \leqslant \|T^{(n+2-s)}P_{|\alpha|\leqslant a}\|$. Thus,

$$\|\psi_{n-1}^{(j)}\| \leqslant C_7 \sum_{s=2}^{n-1} |\mathcal{E}_s|\|\psi_{n-s}^{(j)}\| + C_7 \sum_{s=2}^{n} \|T^{(s+2)}P_{|\alpha|\leqslant a}\|\|\psi_{n-s}\| + C_7\|T^{(3)}P_{|\alpha|\leqslant a}\|\|\psi_{n-1}^{\perp}\|. \tag{43}$$

These inequalities will allow us to obtain upper bounds for the growth of R-S coefficients. In the following theorem we make use of Lemmas 3 and 4.

Theorem 2: *Let k be the number of subspaces as defined in Proposition 3.2. Define $b_1 := C_3[kC_6 + (2+a)^{1/2}]$, $b_2 := 8C_7[b_1C_4 + C_3(2+a)^{1/2} + kC_3C_6]$ and $b_3 := b_1C_4 + C_3C_5[1 + b_2(k-1)]$. Then for any $b \geqslant \max\{b_1, b_2, b_3, 1\}$ and for $n = 1,2,\ldots,$*

$$|\mathcal{E}_n| \leqslant b_1 \kappa^{3n} b^{n-2}[(a+n)!]^{1/2}, \tag{44}$$

$$\|\psi_{n-1}^{(l)}\| \leqslant b_2 \kappa^{3(n-1)} b^{n-2}[(a+n)!]^{1/2}, \tag{45}$$

$$\|\psi_n^{\perp}\| \leqslant b_3 \kappa^{3n} b^{n-2}[(1+a+n)!]^{1/2}. \tag{46}$$

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

$$\|\psi_s\| \leqslant [b_3 + b_2(k-1)]\kappa^{3s} b^{s-1}[(1+a+s)!]^{1/2} \leqslant \kappa^{3s} k b^s [(1+a+s)!]^{1/2} \tag{47}$$

for $s \leqslant n-2$. We shall use the second inequality in (47) to prove (44) and (45), and the first one to prove (46).

Let us start showing (44). Applying Lemmas 3 and 4, statement 2, we obtain

$$\begin{aligned}\sum_{s=2}^{n} \|T^{(s+2)}P_{|\alpha|\leqslant a}\|\|\psi_{n-s}\| &\leqslant C_3 k \sum_{s=2}^{n} \kappa^{s/2}\left[\frac{(1+a+s)!}{(1+a)!}\right]^{1/2} \kappa^{3(n-s)} b^{n-s}[(1+a+n-s)!]^{1/2} \\ &\leqslant C_3 k \kappa^{3n} b^{n-2}[(a+n)!]^{1/2} \sum_{s=2}^{n} \kappa^{-5s/2}\left[\frac{(1+a+s)!(1+a+n-s)!}{(1+a)!(a+n)!}\right]^{1/2} \\ &\leqslant kC_3C_6 \kappa^{3n} b^{n-2}[(a+n)!]^{1/2}.\end{aligned}$$

Thus, (41) yields

$$\begin{aligned}|\mathcal{E}_n| &\leqslant kC_3C_6\kappa^{3n}b^{n-2}[(a+n)!]^{1/2} + C_3\kappa^{3(n-1)}b_3b^{n-3}\kappa^{1/2}(2+a)^{1/2}[(a+n)!]^{1/2} \\ &\leqslant kC_3C_6\kappa^{3n}b^{n-2}[(a+n)!]^{1/2} + C_3(2+a)^{1/2}\kappa^{3n}b^{n-2}[(a+n)!]^{1/2} \\ &\leqslant b_1\kappa^{3n}b^{n-2}[(a+n)!]^{1/2},\end{aligned}$$

which completes the proof of (44).

To prove (45) we start from (43) and proceed in the same fashion:

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$$\|\psi_{n-1}^{(j)}\| \leqslant C_7\kappa^{3n}b_1b_2b^{n-3}\sum_{s=2}^{n-1}[(a+s)!(1+a+n-s)!]^{1/2}+C_3C_7\kappa^{3n}b_3b^{n-3}(2+a)^{1/2}$$
$$\times[(a+n)!]^{1/2}+C_3C_7k\kappa^{3n}b^{n-2}\sum_{s=2}^{n}\kappa^{-5s/2}\left[\frac{(1+a+s)!(1+a+n-s)!}{(1+a)!}\right]^{1/2}$$
$$\leqslant C_7b_1\kappa^{3n}b^{n-2}[(a+n)!]^{1/2}\sum_{m=1}^{n-2}\left[\frac{(1+a+m)!(a+n-m)!}{(a+n)!}\right]^{1/2}$$
$$+C_3C_7(2+a)^{1/2}\kappa^{3n}b^{n-2}[(a+n)!]^{1/2}$$
$$+C_3C_7k\kappa^{3n}b^{n-2}[(a+n)!]^{1/2}\sum_{s=2}^{n}\kappa^{-5s/2}\left[\frac{(1+a+s)!(1+a+n-s)!}{(1+a)!(a+n)!}\right]^{1/2},$$

where we have changed index $s\to m=s-1$ in the first term. From this and statements 1 and 3 of Lemma 4, we obtain

$$\|\psi_{n-1}^{(j)}\| \leqslant 8C_7[b_1C_4+C_3(2+a)^{1/2}+kC_3C_6]\kappa^{3(n-1)}b^{n-2}[(a+n)!]^{1/2}$$
$$=b_2\kappa^{3(n-1)}b^{n-2}[(a+n)!]^{1/2},$$

so (45) is done. Consequently, (47) must be valid for $s=n-1$.

Finally, let us show (46). Note that the first term of (42) is bounded like the first term of (43). Applying statement 2 of Lemma 4, it follows that

$$\|\psi_n^{\perp}\| \leqslant b_1b_3\kappa^{3n}b^{n-3}C_6[(a+n)!]^{1/2}+C_3[1+b_2(k-1)]\kappa^{3n}b^{n-2}[(1+a$$
$$+n)!]^{1/2}\sum_{s=1}^{n}\kappa^{-5s/2}\left[\frac{(1+a+3n-2s)!(1+a+n-s)!}{(1+a+3n-3s)!(1+a+n)!}\right]^{1/2}$$
$$\leqslant b_1C_6\kappa^{3n}b^{n-2}[(1+a+n)!]^{1/2}+C_3[1+b_2(k-1)]C_5\kappa^{3n}b^{n-2}[(1+a+n)!]^{1/2}$$
$$=b_3\kappa^{3n}b^{n-2}[(1+a+n)!]^{1/2}.$$

□

Corollary 1:

$$|\mathcal{E}_n| \leqslant \kappa^{3n}b^{n-1}[(a+n)!]^{1/2},$$

$$\|\psi_n\| \leqslant \kappa^{3n}kb^n[(1+a+n)!]^{1/2}.$$

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 $n\geqslant 3$, in addition to those already defined in the last subsection. Now ψ_0 would be required to lie in a certain subspace $G_{i_1,1_2}\subset G_{i_1}\subset G$, and one would be able to determine ψ_n module an arbitrary component in $G_{i_1,1_2}$. 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,

$$|\mathcal{E}_n| \leqslant \kappa^{3n}b^{n+w}[(1+a+n)!]^{1/2},$$

$$\|\psi_n\| \leqslant \kappa^{3n}b^{n+w}[(1+a+n)!]^{1/2},$$

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

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IV. THE TWO-SIDE ERROR FUNCTION

The upper bounds for $|\mathcal{E}_n|$ and $\|\psi_n\|$ will allow us to estimate the error made in the Schrödinger equation when truncated series are inserted on it. Here we basically follow the technique developed by Hagedorn and Joye in Ref. 4. Concretely, for $N\geqslant 1$ define

$$E_N := e + \sum_{n=1}^{N-1} \hbar^{n/2}\mathcal{E}_n, \quad \Psi_N(x) := \psi_0(x) + \sum_{n=1}^{N-1} \hbar^{n/2}\psi_n(x).$$

These are the truncations at order N of the R-S series. We define

$$\xi_N(x) := A_e[H_0 + W(\hbar;x) - E_N]A_e\Psi_N(x) = \left[H_e + A_eW(\hbar;x)A_e - \sum_{j=1}^{N-1} \hbar^{j/2}\mathcal{E}_jA_e^2\right]\sum_{m=0}^{N-1} \hbar^{m/2}\psi_m(x). \tag{48}$$

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 number of cancellations. The calculation is outlined in the Appendix. The result is

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

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

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

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

$$\xi_N(x) = \hbar^{N/2}\sum_{n=0}^{N-1} \sum_{|\alpha|=N-n+2} \frac{D^\alpha V(\zeta_n)}{\alpha!}A_ex^\alpha A_e\psi_n(x) - \sum_{n=N}^{2N-2} \hbar^{n/2} \sum_{l=n-N+1}^{N-1} \mathcal{E}_lA_e^2\psi_{n-l}(x). \tag{49}$$

Our main result in the next section relies on an upper bound of the L^2-norm of $(H-E_N)A_e\psi_N = A_e^{-1}\xi_N$. Note that, for each $N\geqslant 2$, ξ_N is in the domain of the unbounded operator A_e^{-1}. This estimate on the two-side error function is stated as follows:

Theorem 3: *There are positive constants A, B and N_0 so that*

$$\|A_e^{-1}\xi_N(x)\| \leqslant \sum_{n=N}^{2N} AB^N\hbar^{N/2}[(2+a+n)!]^{1/2}$$

whenever $N_0 \leqslant N$ and $\hbar \leqslant 1$.

To estimate the norm of $A_e^{-1}\xi_N$, we first set a suitable closed region around the bottom of the potential well. 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 $V(x)$. For that reason we shall summarize it as a separate lemma. Here the hypothesis H5 becomes crucial.

For $R>0$, let us define

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

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Lemma 5: Set $R=\sqrt{6N+2a+d-4}$. *Given a multi-index* α, *with* $|\alpha|\geqslant 2$, *and* $n=0,\ldots,N-1$, *there exists certain constants* C_8 *and* C_9 *such that*

$$\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^{\alpha}V(\zeta_n)x^{\alpha'}(1-\chi_R)P_{|\beta|\leqslant a+3n+1}\right\|$$
$$\leqslant C_8 C_9^{(3n+2+a)/2}\frac{(3n+a+d)^{(d-1)/2}}{\left(1-\dfrac{\tau}{\omega_0}\right)^{|\alpha|/2}}\left[\frac{(3n+|\alpha|+[\![d/2]\!]+a)!}{(3n+a)!}\right]^{1/2},$$

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

Proof: Since $|\zeta_n|\leqslant|x|$, the first part of Lemma 3 implies

$$\frac{\delta^{|\alpha|}}{\alpha!}|D^{\alpha}V(\zeta_n)|\leqslant C_0\exp(2\tau x^2). \tag{50}$$

Let us consider an eigenfunction $\Phi_\beta(x)$ of H_0. We have

$$\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^{\alpha}V(\zeta)x^{\alpha'}(1-\chi_R)\Phi_\beta(x)\right\|^2=\int_{\mathbb{R}^d}\left|\frac{\delta^{|\alpha|}}{\alpha!}D^{\alpha}V(\zeta)\right|^2 x^{2\alpha'}|\Phi_\beta(x)|^2[1-\chi_R(x)]d^dx$$
$$\leqslant C_0^2\int_{\mathbb{R}^d}e^{4\tau x^2}x^{2\alpha'}|\Phi_\beta(x)|^2[1-\chi_R(x)]d^dx,$$

where we have dropped the index n in ζ_n. Now change variables $x_i\rightarrow y_i=\sqrt{\omega_i}x_i$ to get

$$\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^{\alpha}V(\zeta)x^{\alpha'}(1-\chi_R)\Phi_\beta(x)\right\|^2$$
$$\leqslant C_0^2\left(\prod_{i=1}^{d}\omega_i^{-\alpha_i'-1/2}\right)\int_{\mathbb{R}^d}e^{\Sigma_i 4(\tau/\omega_i)y_i^2}y^{2\alpha'}|\Phi_\beta(y)|^2[1-\chi_R(y)]d^dy$$
$$\leqslant C_0^2\left(\prod_{i=1}^{d}\omega_i^{-\alpha_i'-1/2}\right)\int_{\mathbb{R}^d}e^{4(\tau/\omega_0)y^2}y^{2\alpha'}|\Phi_\beta(y)|^2[1-\chi_R(y)]d^dy$$
$$=D_1^2\left\|e^{2(\tau/\omega_0)y^2}y^{\alpha'}(1-\chi_R)\Phi_\beta(y)\right\|^2, \tag{51}$$

where D_1 is defined in the obvious way. In the new variables

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

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

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

with energy $e_\beta=|\beta|+d/2$. For $d\geqslant 2$ this operator is equal to

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

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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

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

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 $\nu_q \leqslant C_d e^{\mu_d q}$. This bound suffices for the purpose of our proof. $L_k^j(x)$ denotes the Laguerre polynomial. By Lemma 6.2 of Ref. 4, this polynomial satisfies $|L_k^{q+d/2-1}(x)| \leqslant x^k/k!$ for all $x>4k+2q+d$. Finally, by equating the expressions for the energy, we obtain $|\beta|=2k+q$.

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

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

with $\Sigma|c_{k,q,\nu}|^2=1$. From (51), it follows that

$$\begin{aligned}\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^\alpha V(\zeta)x^{\alpha'}(1-\chi_R)\Phi_\beta(x)\right\|^2 &\leqslant D_1^2 \sum_{\substack{k,q,\nu:\\ 2k+q=|\beta|}} \left\| e^{2(\tau/\omega_0)y^2} y^{\alpha'}(1-\chi_R)\Psi_{k,q,\nu}(y)\right\|^2 \\ &\leqslant D_1^2 \sum_{\substack{k,q,\nu:\\ 2k+q=|\beta|}} \frac{2k!A_{d-1}}{\Gamma(k+q+d/2)}\int_R^\infty e^{-(1-4\tau/\omega_0)r^2} r^{2(|\alpha|-1+q)} \\ &\quad \times |L_k^{q+d/2-1}(r^2)|^2 r^{d-1}dr,\end{aligned}$$

where A_{d-1} is the area of the $(d-1)$ dimensional unit sphere. We also have used that $y^{2|\alpha'|}\leqslant r^{2|\alpha'|}=r^{2(|\alpha|-1)}$. Since $R\geqslant\sqrt{2|\alpha|+d}$, Lemma 6.2 of Ref. 4 applies so

$$\begin{aligned}&\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^\alpha V(\zeta)x^{\alpha'}(1-\chi_R)\Phi_\beta(x)\right\|^2 \\ &\leqslant D_1^2 \sum_{\substack{k,q,\nu:\\ 2k+q=|\beta|}} \frac{2A_{d-1}}{k!\Gamma(k+q+d/2)}\int_R^\infty e^{-(1-4\tau/\omega_0)r^2} r^{2|\alpha|+2q+4k+d-3}dr \\ &= D_1^2 \sum_{\substack{k,q,\nu:\\ 2k+q=|\beta|}} \frac{2A_{d-1}}{k!\Gamma(k+q+d/2)}\frac{\Gamma(|\alpha|+q+2k+d/2-1)}{2(1-4\tau/\omega_0)^{|\alpha|+q+2k+d/2-1}} \\ &= D_1^2 A_{d-1}\frac{\Gamma(|\alpha|+|\beta|+d/2-1)}{(1-4\tau/\omega_0)^{|\alpha|+|\beta|+d/2-1}} \sum_{\substack{k,q:\\ 2k+q=|\beta|}} \frac{\nu_q}{k!\Gamma(k+q+d/2)} \\ &= D_1^2 A_{d-1}\frac{\Gamma(|\alpha|+|\beta|+d/2-1)}{(1-4\tau/\omega_0)^{|\alpha|+|\beta|+d/2-1}} \sum_{k=0}^{[\![|\beta|/2]\!]} \frac{\nu_{|\beta|-2k}}{k!\Gamma(|\beta|-k+d/2)} \\ &\leqslant D_1^2 A_{d-1}C_d e^{\mu_d|\beta|}\frac{\Gamma(|\alpha|+|\beta|+d/2-1)}{(1-4\tau/\omega_0)^{|\alpha|+|\beta|+d/2-1}} \sum_{k=0}^{[\![|\beta|/2]\!]} \frac{e^{-2\mu_d k}}{k!\Gamma(|\beta|-k+d/2)}. \end{aligned} \tag{52}$$

For $|\beta|\geqslant 1$, $|\beta|-k+d/2\geqslant 1+d/2\geqslant 2$ for all $0\leqslant k\leqslant[\![|\beta|/2]\!]$. Since $\Gamma(x)$ is an increasing function for $x\geqslant 2$, we have

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$$\sum_{k=0}^{[\![|\beta|/2]\!]} \frac{e^{-2\mu_d k}}{k!\Gamma(|\beta|-k-d/2)} \leqslant \sum_{k=0}^{[\![|\beta|/2]\!]} \frac{1}{k!(|\beta|-k)!} \leqslant \frac{1}{|\beta|!}\sum_{k=0}^{|\beta|}\binom{|\beta|}{k} = \frac{1}{|\beta|!}2^{|\beta|}.$$

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

$$\sum_{k=0}^{[\![|\beta|/2]\!]} \frac{e^{-2\mu_d k}}{k!\Gamma(|\beta|-k-d/2)} \leqslant \frac{2}{\sqrt{\pi}|\beta|!}2^{|\beta|}$$

for all $|\beta|\geqslant 0$. Thus (52) becomes

$$\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^\alpha V(\zeta)x^{\alpha'}(1-\chi_R)\Phi_\beta(x)\right\|^2 \leqslant D_2^2 2^{|\beta|}e^{\mu_d|\beta|}\frac{\Gamma(|\alpha|+|\beta|+d/2-1)}{|\beta|!(1-4\tau/\omega_0)^{|\alpha|+|\beta|+d/2-1}}$$

with $D_2^2 := 2D_1^2 A_{d-1}C_d\pi^{-1/2}$.

Now consider any $\varphi\in\mathrm{Ran}(P_{|\beta|\leqslant 3n+a+1})$ so $\varphi=\Sigma_{|\beta|\leqslant 3n+a+1}c_\beta\Phi_\beta(x)$. Then the Hölder inequality implies that

$$\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^\alpha V(\zeta)x^{\alpha'}(1-\chi_R)P_{|\beta|\leqslant a+3n+1}\varphi\right\|^2 \leqslant \|\varphi\|^2\sum_{|\beta|\leqslant 3n+a+1}\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^\alpha V(\zeta)x^{\alpha'}(1-\chi_R)\Phi_\beta(x)\right\|^2.$$

Therefore

$$\begin{aligned}\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^\alpha V(\zeta)x^{\alpha'}(1-\chi_R)P_{|\beta|\leqslant a+3n+1}\right\|^2 &\leqslant D_2^2\frac{2^{3n+a+1}e^{\mu_d(3n+a+1)}}{\left(1-\frac{4\tau}{\omega_0}\right)^{3n+|\alpha|+a+d/2}}\sum_{|\beta|\leqslant 3n+a+1}\frac{\Gamma(|\alpha|+|\beta|+d/2-1)}{|\beta|!}\\ &\leqslant D_2^2\frac{2^{3n+a+1}e^{\mu_d(3n+a+1)}}{(1-4\tau/\omega_0)^{3n+|\alpha|+a+d/2}}\sum_{|\beta|\leqslant 3n+a+1}\frac{(|\alpha|+|\beta|+[\![d/2]\!]-1)!}{|\beta|!}\end{aligned}$$

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

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

and, moreover, $(3n+2+a)/(3n+1+a)\leqslant 2$. Thus,

$$\begin{aligned}\left\|\frac{\delta^{|\alpha|}}{\alpha!}D^\alpha V(\zeta)x^{\alpha'}(1-\chi_R)P_{|\beta|\leqslant a+3n+1}\right\|^2 \\ \leqslant D_2^2\frac{2^{3n+a+2}e^{\mu_d(3n+a+1)}}{(1-4\tau/\omega_0)^{3n+|\alpha|+a+d/2}}(3n+a+d)^{d-1}\frac{(3n+|\alpha|+[\![d/2]\!]+a)!}{(3n+a)!}.\end{aligned}$$

Now define $C_8 := D_2 e^{-\mu_d/2}(1-4\tau/\omega_0)^{1-d/4}$ and $C_9 := [2e^{\mu_d}/(1-4\tau/\omega_0)]^{1/2}$. □

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Proof of Theorem 3: Recall that we assume that $\delta \leqslant 1$. We already know, from Theorem 2, that $b \geqslant 1$. From the proof of Lemma 3, we also know that $\|x_i A_e\| \leqslant \gamma$. Now, from (49), it follows that

$$\begin{aligned}
\|A_e^{-1}\xi_N(x)\| &\leqslant \hbar^{N/2}\sum_{n=0}^{N-1}\sum_{|\alpha|=N-n+2}\left\|\frac{D^\alpha V(\zeta_n)}{\alpha!}(1-\chi_R(x))x^\alpha A_e\psi_n(x)\right\| \\
&\quad + \hbar^{N/2}\sum_{n=0}^{N-1}\sum_{|\alpha|=N-n+2}\left\|\frac{D^\alpha V(\zeta_n)}{\alpha!}\chi_R(x)x^\alpha A_e\psi_n(x)\right\| \\
&\quad + \sum_{n=N}^{2N-2}\hbar^{n/2}\sum_{l=n-N+1}^{N-1}\|\mathcal{E}_l A_e\psi_{n-l}(x)\| \\
&\leqslant \hbar^{N/2}\sum_{n=0}^{N-1}\sum_{|\alpha|=N-n+2}\left\|\frac{D^\alpha V(\zeta_n)}{\alpha!}(1-\chi_R(x))x^{\alpha'}P_{|\beta|\leqslant 3n+a+1}\right\|\|x_iA_e\|\|\psi_n(x)\| \\
&\quad + \hbar^{N/2}\sum_{n=0}^{N-1}\sum_{|\alpha|=N-n+2}\left\|\frac{D^\alpha V(\zeta_n)}{\alpha!}\chi_R(x)x^{\alpha'}P_{|\beta|\leqslant 3n+a+1}\right\|\|x_iA_e\|\|\psi_n(x)\| \\
&\quad + \sum_{n=N}^{2N-2}\hbar^{n/2}\sum_{l=n-N+1}^{N-1}|\mathcal{E}_l|\|\psi_{n-l}(x)\|, \qquad (53)
\end{aligned}$$

where we split x^α into $x^{\alpha'}x_i$, which is possible for some coordinate x_i because $|\alpha| \geqslant 2$. Then $|\alpha'| = |\alpha|-1$. Let us estimate each term on the right hand side of (53) individually. Applying Lemma 5 and the estimates for $\|x_\alpha A_e\|$ and $\|\psi_n\|$, we obtain

$$\begin{aligned}
\text{first term} &\leqslant \hbar^{N/2}\sum_{n=0}^{N-1}\sum_{|\alpha|=N+2-n}\delta^{|\alpha|}C_8C_9^{(3n+a+2)/2}\left(1-\frac{4\tau}{\omega_0}\right)^{-|\alpha|/2}(3n+a+d)^{(d-1)/2} \\
&\quad \times \left[\frac{(3n+|\alpha|+[\![d/2]\!]+a)!}{(3n+a)!}\right]^{1/2}\gamma\kappa^{3n}b^{n+w}[(1+a+n)!]^{1/2} \\
&\leqslant C_8\gamma\hbar^{N/2}b^{N+w}\delta^{-(N+2)}C_9^{(3N+a+d+1)/2}\left(1-\frac{4\tau}{\omega_0}\right)^{-(N+2)/2}(3N+a+d-3)^{(d-1)/2} \\
&\quad \times \sum_{n=0}^{N-1}\kappa^{3n}\left[\frac{(2n+N+[\![d/2]\!]+a+2)!(n+a+1)!}{(3n+a)!}\right]^{1/2}\sum_{|\alpha|=N+2-n}1.
\end{aligned}$$

From the proof of Lemma 2, we know that $\Sigma_{|\alpha|=N+2-n}1 \leqslant [(d-1)!]^{-1}(N+d+1)^{d-1}$. Let us define $A_1 := \gamma\delta^{-2}b^wC_8C_9^{(a+d+1)/2}[(d-1)!(1-4\tau/\omega_0)]^{-1}$ and $B_1 := \delta^{-1}C_9^{3/2}b(1-4\tau/\omega_0)^{-1}$. Then

$$\begin{aligned}
\text{first term} &\leqslant A_1B_1^N\hbar^{N/2}(N+d+1)^{d-1}(3N+a+d-3)^{(d-1)/2} \\
&\quad \times \sum_{n=0}^{N-1}\kappa^{3n}\left[\frac{(2n+N+[\![d/2]\!]+a+2)!(n+a+1)!}{(3n+a)!}\right]^{1/2}.
\end{aligned}$$

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

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$$\text{first term} \leqslant A_1 B_1^N \hbar^{N/2} (3N+a+d-3)^{(d-1)/2} (N+d+1)^{d-1} (3N+a+[\![d/2]\!])^{[\![d/2]\!]/2} \times [(2+a+N)!]^{1/2} \sum_{n=0}^{N-1} \kappa^{3n} \left[\frac{(2+a+N+2n)!(1+a+n)!}{(a+3n)!(2+a+N)!} \right]^{1/2}$$

$$\leqslant A_1 B_1^N \kappa^{3N} \hbar^{N/2} (3N+a+d-3)^{(d-1)/2} (N+d+1)^{d-1} (3N+a+[\![d/2]\!])^{[\![d/2]\!]/2} \times [(2+a+N)!]^{1/2} \max_{1\leqslant l \leqslant N} \left[\frac{(3N-3l+a+1)(3N-3l+a+2)}{(N-l+a+2)} \right]^{1/2} \times \sum_{l=1}^{N} \kappa^{-5l/2} \left[\frac{(2+a+3N+2l)!(2+a+N-l)!}{(2+a+3N-3l)!(2+a+N)!} \right]^{1/2}.$$

The change of index $n \to l = N-n$ was performed in the last sumation above. Now we need to apply Lemma 4, statement 2, to obtain

$$\text{first term} \leqslant C_5 A_1 B_1^N \kappa^{3N} \hbar^{N/2} (3N+a+d-3)^{(d-1)/2} (N+d+1)^{d-1} (3N+a+[\![d/2]\!])^{[\![d/2]\!]/2} \times [3(3N+a+2)]^{1/2} [(2+a+N)!]^{1/2}.$$

Finally, define N_1 as the smallest integer such that the inequality

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

holds for all $N \geqslant N_1$. Then, whenever $N \geqslant N_1$,

$$\text{first term} \leqslant C_5 A_1 B_1^N \kappa^{4N} \hbar^{N/2} [(2+a+N)!]^{1/2}.$$

Statement 2 of Lemma 2 yields

$$\frac{\delta^{|\alpha|}}{\alpha!} |D^\alpha V(\zeta(x))| \leqslant C_0 \exp\left(\frac{2\tau d}{\omega_0^2} R^2 \right) = C_0 \exp\left[\frac{2\tau d}{\omega_0^2} (2a+d-4) \right] \exp\left(\frac{12\tau d}{\omega_0^2} N \right)$$

on the support of $\chi_R(x)$. Thus, the second term of (53) satisfies

$$\text{second term} \leqslant \hbar^{N/2} \gamma \delta^{-(N+2)} C_0 \exp\left[\frac{2\tau d}{\omega_0^2} (2a+d-4) \right] \exp\left(\frac{12\tau d}{\omega_0^2} N \right) \times \sum_{n=0}^{N-1} \sum_{|\alpha|=N-n+2} \| x^{\alpha'} P_{|\beta| \leqslant 3n+a+1} \| \| \psi_n(x) \|$$

$$\leqslant \hbar^{N/2} \gamma \delta^{-(N+2)} C_0 \exp\left[\frac{2\tau d}{\omega_0^2} (2a+d-4) \right] \exp\left(\frac{12\tau d}{\omega_0^2} N \right) \times \sum_{n=0}^{N-1} \sum_{|\alpha|=N-n+2} \kappa^{(|\alpha|-1)/2} \left[\frac{(a+|\alpha|+3n)!}{(1+a+3n)!} \right]^{1/2} \kappa^{3n} b^{n+w} [(1+a+n)!]^{1/2}$$

$$\leqslant \hbar^{N/2} \gamma \delta^{-(N+2)} C_0 \exp\left[\frac{2\tau d}{\omega_0^2} (2a+d-4) \right] \exp\left(\frac{12\tau d}{\omega_0^2} N \right) b^{N+w} \kappa^{(N+1)/2} \times \sum_{n=0}^{N-1} \kappa^{5n/2} \left[\frac{(2+a+N+2n)!(1+a+n)!}{(1+a+3n)!} \right]^{1/2} \sum_{|\alpha|=N-n+2} 1.$$

Define $A_2 := \gamma \delta^{-2} \kappa^{1/2} C_0 b^w \exp[2\tau d(2a+d-4)][(d-1)!]^{-1}$ and $B_2 := \delta^{-1} \kappa^{1/2} b \exp(12\tau d/\omega_0^2)$. Then, following the argument we have used to estimate the first term, we obtain

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$$\text{second term} \leqslant A_2 B_2^N \hbar^{N/2} (N+d+1)^{d-1} \sum_{n=0}^{N-1} \kappa^{3n} \left[\frac{(2+a+N+2n)!(1+a+n)!}{(1+a+3n)!} \right]^{1/2}$$

$$\leqslant A_2 B_2^N \kappa^{3N} \hbar^{N/2} (N+d+1)^{d-1} [(2+a+N)!]^{1/2}$$

$$\times \max_{1 \leqslant l \leqslant N} \left[\frac{2+a+3N-3l}{2+a+N-l} \right]^{1/2} \sum_{l=1}^{N} \kappa^{-5l/2} \left[\frac{(2+a+3N+2l)!(2+a+N-l)!}{(2+a+3N-3l)!(2+a+N)!} \right]^{1/2}$$

$$\leqslant 3^{1/2} C_5 A_2 B_2^N \kappa^{3N} \hbar^{N/2} (N+d+1)^{d-1} [(2+a+N)!]^{1/2}.$$

Now define N_2 such that $(N+d+1)^{d-1} \leqslant \kappa^N$ for every $N \geqslant N_2$. Then

$$\text{second term} \leqslant 3^{1/2} C_5 A_2 B_2^N \kappa^{4N} \hbar^{N/2} [(2+a+N)!]^{1/2}.$$

For the third term of (53), we only need to use the first statement of Lemma 4. The result is

$$\text{third term} \leqslant \sum_{n=N}^{2N} C_4 \kappa^{3n} b^{n+2w} \hbar^{N/2} [(1+a+n)!]^{1/2}.$$

To complete the proof define $N_0 = \max\{N_1, N_2\}$, $A = \max\{C_5 A_1, 3^{1/2} C_5 A_2, C_4 b^{2w}\}$ and $B = \max\{\kappa^4 B_1, \kappa^3 B_2, \kappa^3 b\}$. □

V. OPTIMAL TRUNCATION

In this section we shall 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 shall use our estimate of the norm $A_e^{-1}\xi_N(x)$. We shall 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.

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,

$$E(\hbar) \sim e + \mathcal{E}_1 \hbar^{1/2} + \ldots + \mathcal{E}_{M-1} \hbar^{(M-1)/2} + \mathcal{E}_M \hbar^{M/2} + \mathcal{E}_{M+1} \hbar^{(M+1)/2} + \ldots,$$

$$E'(\hbar) \sim e + \mathcal{E}_1 \hbar^{1/2} + \ldots + \mathcal{E}_{M-1} \hbar^{(M-1)/2} + \mathcal{E}'_M \hbar^{M/2} + \mathcal{E}'_{M+1} \hbar^{(M+1)/2} + \ldots,$$

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

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

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

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

whenever $\hbar \leqslant \hbar_a(M)$. Then

$$|E(\hbar) - E'(\hbar)| \geqslant |\mathcal{E}_M - \mathcal{E}'_M| \hbar^{M/2} - C_M \hbar^{(M+1)/2}.$$

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

$$C_M \hbar^{(M+1)/2} \leqslant \tfrac{1}{2} |\mathcal{E}_M - \mathcal{E}'_M| \hbar^{M/2}.$$

Thus for $\hbar \leqslant \hbar_1 := \min\{\hbar_a(M), \hbar_b(M)\}$ we have

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$$|E(\hbar)-E'(\hbar)|\geq \tfrac{1}{2}|\mathcal{E}_M-\mathcal{E}'_M|\hbar^{M/2}.$$

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

Lemma 6: Let $E(\hbar)$ and $E'(\hbar)$ be distinct eigenvalues of $H(\hbar)$, which degenerate at $\hbar=0$. Then either

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

(2) there exists M and $\hbar_1=\hbar_1(M)$ such that

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

whenever $\hbar\leq\hbar_1$.

Remark: It is clear that Lemma 6 is also valid when several eigenvalues of $H(\hbar)$ converge 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 7: Suppose $\Sigma_{n=0}f_n\beta^n$ 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

$$\left| f(\beta)-\sum_{n=0}^{N-1} f_n\beta^n\right| \leq \epsilon\beta^M \tag{54}$$

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

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

$$\beta_1(N)<\min\{(\epsilon C_N^{-1})^{1/(N-M)},\beta_1(N-1)\}.$$

Then

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

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

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

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

Then (54) holds whenever $N_0\leq N\leq N(\beta)$. □

Let $\{e_I\}_{I=0}^{\infty}$ be an arrangement in increasing order of the eigenvalues of H_0, counting multiplicities. Theorem 1.1 of Ref. 16 states that given a non-negative integer J, we can choose $\hbar_0$ so that for each $\hbar\leq\hbar_0$ there are at least $J+K$ eigenvalues of $H(\hbar)$, counting multiplicities. Furthermore, each one of them converges to one of the first $J+K$ eigenvalues of H_0. In the following proposition, we study the behavior of truncations of the R-S series of $E^J(\hbar)$, the Jth eigenvalue of $H(\hbar)$. We set K so that $e_{J+K}>e_J$.

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Proposition 3: Let $E(\hbar)=E^J(\hbar)$ *be a non-quasi-degenerate eigenvalue of* $H(\hbar)$*, which converges to* $e=e_J$*. 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, for each* $\hbar\leqslant\hbar_e$ *there is an* $N_e(\hbar)\geqslant N_0$ *such that*

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

for all $N_0\leqslant N\leqslant N_e(\hbar)$.

Proof: We shall consider the case where there exists another eigenvalue of $H(\hbar)$ that converges to e. The proof can be easily simplified to accomodate the opposite situation, which is studied in Proposition 3 of Ref. 19. So said, let $E'(\hbar)$ be another eigenvalue of $H(\hbar)$ converging to e as $\hbar\searrow 0$. By Lemma 6, there are M and $\hbar_1$ so that $|E(\hbar)-E'(\hbar)|\geqslant\frac{1}{2}|\Delta\mathcal{E}_M|\hbar^{M/2}$ for $\hbar\leqslant\hbar_1$. Without loss we may assume that $N_0\geqslant M$. To simplify the proof, we furthermore assume that no other eigenvalue of $H(\hbar)$ converges to e. Let G_e be the eigenspace associated to e.

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

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

Then, from Theorem 3 it follows that

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

whenever $\hbar\leqslant\hbar_0:=\min\{1,|\Delta\mathcal{E}_M|^{-2/M}\}$ and $N_0\leqslant N\leqslant N_1(\hbar)$. On the other hand, note that $\Psi_N=\psi_0+\varphi_N$, where φ_N is orthogonal to $\psi_0\in G_e$ because of the normalization we chose for the correction terms ψ_n. Since $A_e\psi_0=\psi_0$, we conclude that $\|A_k\Psi_N(\hbar;x)\|\geqslant 1$. So Theorem 3 implies that

$$\|[H(\hbar)-E_N(\hbar)]A_e\Psi_N(\hbar;x)\|\leqslant\sum_{n=N}^{2N}AB^n\hbar^{n/2}[(2+a+n)!]^{1/2}\|A_e\Psi_N(\hbar;x)\|. \tag{55}$$

We may assume that $E_N(\hbar)\notin\sigma(H(\hbar))$, so $[H(\hbar)-E_N(\hbar)]$ is invertible. It follows that

$$\left\{\sum_{n=N}^{2N}AB^n\hbar^{n/2}[(2+a+n)!]^{1/2}\right\}^{-1}\leqslant\|[H(\hbar)-E_N(\hbar)]^{-1}\|.$$

Because H is self-adjoint, $\|(H-E)^{-1}\|=\mathrm{dist}\{E,\sigma(H)\}^{-1}$ by the spectral theorem. Thus,

$$\mathrm{dist}\{E_N(\hbar),\sigma(H)\}\leqslant\sum_{n=N}^{2N}AB^n\hbar^{n/2}[(2+a+n)!]^{1/2}\leqslant\frac{1}{4}|\Delta\mathcal{E}_M|\hbar^{M/2} \tag{56}$$

for $\hbar\leqslant\hbar_0$ and $N_0\leqslant N\leqslant N_1(\hbar)$. Let Δ be the minimum nonzero distance between the first $J+K$ eigenvalues of H_0. Since $E_I(\hbar)\to e_I$, we can set $\hbar_\Delta>0$ so that for $0\leqslant I\leqslant J+K$, $|E_I(\hbar)-e_I|\leqslant\frac{1}{4}\Delta$ if $\hbar\leqslant\hbar_\Delta$. That implies that, for $\hbar\leqslant\hbar_\Delta$ and $E''(\hbar)\in\sigma(H(\hbar))\backslash\{E(\hbar),E'(\hbar)\}$,

$$|E^{\#}(\hbar)-E''(\hbar)|\geqslant\tfrac{1}{2}\Delta$$

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

$$|E(\hbar)-E''(\hbar)|\geqslant\tfrac{1}{2}|\Delta\mathcal{E}_M|\hbar^{M/2},$$

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$$|E(\hbar)-E'(\hbar)|\geqslant \tfrac{1}{2}|\Delta\mathcal{E}_M|\hbar^{M/2},$$

which ultimately implies that

$$\mathrm{dist}\{E(\hbar),\sigma(H)\backslash E(\hbar)\}\geqslant \tfrac{1}{2}|\Delta\mathcal{E}_M|\hbar^{M/2} \tag{57}$$

whenever $\hbar\leqslant\min\{\hbar_0,\hbar_1,\hbar_\Delta,\hbar_2\}$. Since $E_N(\hbar)$ is asymptotic to $E(\hbar)$, we may apply Lemma 7. Then there is $\hbar_3>0$ such that for each $\hbar\leqslant\hbar_3$ we can fix $N_2(\hbar)\geqslant N_0$ so that

$$|E(\hbar)-E_N(\hbar)|\leqslant \tfrac{1}{4}|\Delta\mathcal{E}_M|\hbar^{M/2} \tag{58}$$

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

Now (57), (58) and the second inequality of (56) imply that

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

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

Remark: The number $N_e(\hbar)$ defined in the proof must indeed be equal to $N_1(\hbar)$. Assume that $N_e(\hbar)<N_1(\hbar)$, and consider $N_e(\hbar)\leqslant N\leqslant N_1(\hbar)$. Then $E_N(\hbar)$ has to be near some eigenvalue $E''(\hbar)$ different to $E(\hbar)$. By reducing $\hbar$, $E_N(\hbar)$ approaches to $E(\hbar)$ while keeping itself close to $E''(\hbar)$, which leads to a contradiction.

Remark: $N_e(\hbar)$ grows like $g/\hbar$, as one can see from the proof of Theorem 4 below.

The requirement of $E(\hbar)$ to be non-quasi-degenerate can be relaxed, and we formulate the following weaker version of Proposition 3. The proof is a straighforward variation of it.

Proposition 4: Let $E(\hbar)=E^J(\hbar)$ be an eigenvalue of $H(\hbar)$, which converges to $e=e_J$. 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 6 [including $E(\hbar)$ itself.] Then there exists $\hbar_e>0$ so that for each $\hbar\leqslant\hbar_e$ there is an $N_e(\hbar)\geqslant N_0$ such that

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

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

In the following theorem we assume the hypotheses of Proposition 3. An analogous result follows from the hypotheses of 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 $\hbar\leqslant\hbar_g$ there exists $N(\hbar)$ such that*

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

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

Proof: Fix $0<g<B^{-2}$. Then $0<B^2g<1$; consequently there is $\Omega>0$ such that $B^2g=\exp(-\Omega)$. Consider the function

$$f(\hbar):=Ag\exp\left(-\frac{\Omega(1+a)}{4}\right)\hbar^{-(4+a+M)/2}\exp\left(-\frac{\Omega g}{4\hbar}\right).$$

It is clear that $f(\hbar)>0$ on $(0,\infty)$ has a single maximum, and $f(\hbar)\to 0$ as $\hbar\to 0$ or $\hbar\to\infty$. Now set

$$\hbar_4=\sup\{\hbar:f(\hbar)\ \text{ is increasing and }\ f(\hbar)\leqslant\tfrac{1}{4}|\Delta\mathcal{E}_M|\}.$$

Then set

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

Now for $\hbar \leqslant \hat{\hbar}_g$ define $N(\hbar)$ by $2+a+2N(\hbar) = [\![g/\hbar]\!]$. So defined, $N(\hbar) \geqslant N_0$. On the other hand, since we can assume $B \geqslant 1$ and $2+a+n \leqslant g/\hbar$ for $N(\hbar) \leqslant n \leqslant 2N(\hbar)$ we have

$$\begin{aligned}\sum_{n=N(\hbar)}^{2N(\hbar)} AB^n \hbar^{n/2}[(2+a+n)!]^{1/2} &\leqslant \sum_{n=N(\hbar)}^{2N(\hbar)} AB^n \hbar^{n/2}(2+a+n)^{(2+a+n)/2}\\ &\leqslant A\hbar^{-(2+a)/2} \sum_{n=N(\hbar)}^{2N(\hbar)} [B^2\hbar(2+a+n)]^{(2+a+n)/2}\\ &\leqslant A\hbar^{-(2+a)/2} \sum_{n=N(\hbar)}^{2N(\hbar)} (B^2 g)^{(2+a+n)/2}.\end{aligned}$$

Now use that $B^2 g = \exp(-\Omega) < 1$ and the fact that $x^n \geqslant x^{n+1}$ if $x \leqslant 1$ to obtain

$$\begin{aligned}\sum_{n=N(\hbar)}^{2N(\hbar)} AB^n \hbar^{n/2}[(2+a+n)!]^{1/2} &\leqslant A\hbar^{-(2+a)/2} \sum_{n=N(\hbar)}^{2N(\hbar)} \exp\left\{-\frac{\Omega}{2}[2+a+N(\hbar)]\right\}\\ &= A\hbar^{-(2+a)/2} e^{-(\Omega/4)(2+a)}[1+N(\hbar)]\exp\left\{-\frac{\Omega}{4}[2+a+2N(\hbar)]\right\}\\ &\leqslant A\hbar^{-(2+a)/2} e^{-(\Omega/4)(2+a)}[2+a+2N(\hbar)]\exp\left[-\frac{\Omega}{4}\left(\frac{g}{\hbar}-1\right)\right]\\ &\leqslant Age^{-(\Omega/4)(1+a)} \hbar^{-(4+a+M)/2} \exp\left(-\frac{\Omega g}{4\hbar}\right)\hbar^{M/2}\\ &\leqslant f(\hbar_4)\hbar^{M/2} \qquad (59)\\ &\leqslant \tfrac{1}{4}|\Delta\mathcal{E}_M|\hbar^{M/2}. \qquad (60)\end{aligned}$$

Thus, $N(\hbar) \leqslant N_e(\hbar)$. Therefore, Proposition 3 holds for $\hbar < \hat{\hbar}_g$, which along with (59) implies

$$|E_{N(\hbar)}(\hbar) - E(\hbar)| \leqslant Age^{-(\Omega/4)(1+a)} \hbar^{-(4+a)/2} \exp\left(-\frac{\Omega g}{4\hbar}\right),$$

for all $\hbar \leqslant \hat{\hbar}_g$. Finally, define

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

Then the assertion is true for all $\hbar \leqslant \hbar_g$ with $\Gamma := \Omega g/8$ and $\Lambda := Ag\exp(-\Omega(1+a)/4)$. □

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

$$\left\|\frac{\tilde{\Psi}_N(\hbar;x)}{\|\tilde{\Psi}_N(\hbar;x)\|} - \frac{P_E\tilde{\Psi}_N(\hbar;x)}{\|P_E\tilde{\Psi}_N(\hbar;x)\|}\right\| \leqslant 16|\Delta\mathcal{E}_M|^{-1} \sum_{n=N}^{2N} AB^n \hbar^{(n-M)/2}[(2+a+n)!]^{1/2}$$

for some $M \leqslant N_0$.

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Proof: Notice that (55) means that

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

On the other hand, we can write

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

where $\Omega_N(\hbar;x)$ is orthogonal to G_E, and $|w_N|^2+\|\Omega_N(\hbar;x)\|^2=1$. Since these functions are defined up to a global phase, we can assume that indeed $0<w_n\leqslant 1$. Then the normalization condition implies

$$\|\Omega_N(\hbar;x)\|\geqslant\|\Omega_N(\hbar;x)\|^2=1-|w_N|^2=(1+w_N)(1-w_N)\geqslant 1-w_N.$$

So we have

$$\|\|\tilde{\Psi}_N(\hbar;x)\|^{-1}\tilde{\Psi}_N(\hbar;x)-\|P_E\tilde{\Psi}_N(\hbar;x)\|^{-1}P_E\tilde{\Psi}_N(\hbar;x)\|\leqslant 2\|\Omega_N(\hbar;x)\|. \tag{61}$$

Since

$$[H(\hbar)-E_N(\hbar)]\Omega_N(\hbar;x)=[H(\hbar)-E_N(\hbar)]\frac{\tilde{\Psi}_N(\hbar;x)}{\|\tilde{\Psi}_N(\hbar;x)\|}-w_N[E(\hbar)-E_N(\hbar)]\frac{P_E\tilde{\Psi}_N(\hbar;x)}{\|P_E\tilde{\Psi}_N(\hbar;x)\|},$$

it follows from Proposition 3 that

$$\|[H(\hbar)-E_N(\hbar)]\Omega_N(\hbar;x)\|\leqslant 2\sum_{n=N}^{2N}AB^n\hbar^{n/2}[(2+a+n)!]^{1/2} \tag{62}$$

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

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

$$\|\Omega_N(\hbar;x)\|\leqslant\|[H(\hbar)-E_N(\hbar)]_\perp^{-1}\|\|[H(\hbar)-E_N(\hbar)]\Omega_N(\hbar;x)\|, \tag{63}$$

where $[H(\hbar)-E_N(\hbar)]_\perp$ is the restriction of $[H(\hbar)-E_N(\hbar)]$ to the subspace orthogonal to G_E. For simplicity, let us assume that there is only one distinct eigenvalue $E'(\hbar)$ that converges to the same eigenvalue of H_0 as $E(\hbar)$. Since

$$\text{dist}\{E_N(\hbar),\sigma(H)\backslash E(\hbar)\}\geqslant\tfrac{1}{2}\text{dist}\{E(\hbar),\sigma(H)\backslash E(\hbar)\},$$

the spectral theorem along with (57) implies that

$$\|[H(\hbar)-E_N(\hbar)]_\perp^{-1}\|\leqslant 4|\Delta\mathcal{E}_M|^{-1}\hbar^{-M/2}. \tag{64}$$

The assertion now follows from (61)–(64). □

Remark: The assumption of non-quasi-degeneracy of $E(\hbar)$ is critical, as one can see in the argument that leads to (64).

The last result of this section concerns the optimal truncation for the eigenfunctions of $H(\hbar)$. It follows from Proposition 5 in the same way as Theorem 4 does from Proposition 3:

Theorem 5: *Fix $0\leqslant g\leqslant B^{-2}$. Let Λ and Γ be defined as in Theorem 4. Then there exists $\hbar_g'>0$ such that for each $\hbar\leqslant\hbar_g'$ there is $N(\hbar)$ so that*

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$$\left\| \frac{\widetilde{\Psi}_{N(\hbar)}(\hbar;x)}{\|\widetilde{\Psi}_{N(\hbar)}(\hbar;x)\|} - \frac{P_E \widetilde{\Psi}_{N(\hbar)}(\hbar;x)}{\|P_E \widetilde{\Psi}_{N(\hbar)}(\hbar;x)\|} \right\| \leqslant 16 |\Delta \mathcal{E}_M| \Lambda \exp\left(-\frac{\Gamma}{\hbar} \right).$$

Proof: Define

$$f'(\hbar) := Ag \exp\left(-\frac{\Omega(1+a)}{4} \right) \hbar^{-(4+a+2M)/2} \exp\left(-\frac{\Omega g}{4\hbar} \right),$$

$$\hbar_4' := \sup\{\hbar : f'(\hbar) \text{ is increasing and } f(\hbar) \leqslant \tfrac{1}{4}|\Delta \mathcal{E}_M|\},$$

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

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

Now proceed as in the proof of Theorem 4. □

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APPENDIX: COMPUTATION OF ξ_N

Here we simplify the formula (48) by using the identity (10). This calculation is formally identical the one done in Ref. 19, with some notational change. We reproduce it here for a sake of convenience:

$$\xi_N = \left[H_e + A_e W A_e - \sum_{j=1}^{N-1} \hbar^{j/2} \mathcal{E}_j A_e^2 \right] \sum_{m=0}^{N-1} \hbar^{m/2} \psi_m$$
$$= \sum_{m=0}^{N-1} \hbar^{m/2} H_e \psi_m + \sum_{m=0}^{N-1} \hbar^{m/2} A_e W A_e \psi_m - \sum_{j=1}^{N-1} \sum_{m=0}^{N-1} \hbar^{(j+m)/2} \mathcal{E}_j A_e^2 \psi_m .$$

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

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

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

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

$$=\sum_{p=0}^{N-1}\sum_{m=p}^{N-1}\hbar^{(p+N)/2}T^{(p+N-m+2)}\psi_m+\sum_{m=0}^{N-1}\hbar^{m/2}A_eW^{[N+2]}A_e\psi_m$$

$$-\sum_{n=N}^{2N-2}\hbar^{n/2}\sum_{j=n-N+1}^{N-1}\mathcal{E}_jA_e^2\psi_{n-j}$$

$$=\sum_{m=0}^{N-1}\hbar^{m/2}\sum_{p=0}^{m}\hbar^{(p+N-m)/2}T^{(p+N-m+2)}\psi_m$$

$$+\sum_{m=0}^{N-1}\hbar^{m/2}A_eW^{[N+2]}A_e\psi_m-\sum_{n=N}^{2N-2}\hbar^{n/2}\sum_{j=n-N+1}^{N-1}\mathcal{E}_jA_e^2\psi_{n-j}$$

$$=\sum_{m=0}^{N-1}\hbar^{m/2}\left[\sum_{i=2}^{m+2}\hbar^{(i+N-m-2)/2}T^{(i+N-m)}+A_eW^{[N+2]}A_e\right]\psi_m-\sum_{n=N}^{2N-2}\hbar^{n/2}\sum_{j=n-N+1}^{N-1}\mathcal{E}_jA_e^2\psi_{n-j}.$$

Finally, note that $\hbar^{(j-2/2)}T^{(j)}+A_eW^{[j+1]}A_e=A_eW^{[j]}A_e$. Therefore, it follows that

$$\xi_N=\sum_{m=0}^{N-1}\hbar^{m/2}A_eW^{[N-m+1]}A_e\psi_m-\sum_{n=N}^{2N-2}\hbar^{n/2}\sum_{j=n-N+1}^{N-1}\mathcal{E}_jA_e^2\psi_{m-j}.$$

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