Numerical analysis of a multiscale finite element scheme for the resolution of the stationary Schrödinger equation

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Abstract

A numerical method for the resolution of the one dimensional Schrödinger equation with open boundary conditions was presented in [N. Ben Abdallah, O. Pinaud, *Improved simulation of open quantum systems: resonances and WKB interpolation schemes*, submitted in J. Comp. Phys.]. The main attribute of this method is a significant reduction of the computational cost for a desired accuracy. It is based particularly on the derivation of WKB basis functions, better suited for the approximation of highly oscillating wave functions than the standard polynomial interpolation functions. The present paper is concerned with the numerical analysis of this method. Consistency and stability results are presented. An error estimate in terms of the mesh size and independent on the wavelength λ is established. This property illustrates the importance of this method, as multi-wavelength grids can be chosen to get accurate results, reducing by this manner the simulation time.

Keywords : Schrödinger equation; Open boundary conditions; WKB approximation; WKB finite element scheme; Consistency; Stability; Convergence.

1 Introduction

The Schrödinger equation is frequently used for the description of the quantum, ballistic electron transport in nanoscale semiconductor devices. A lot of work is dedicated to the numerical simulation of such 2D or 3D devices [6, 7, 17]. In a previous work [4], a numerical method for the resolution of the 1D Schrödinger equation, describing the electron transport in a resonant tunneling diode (RTD) was introduced. This method is based on the self-consistent resolution of the Schrödinger-Poisson system with open boundary conditions [13] and combines two methods to reduce the simulation time. On one hand, the WKB approximation enables the use of coarser space grids. On the other hand, a reduction of the injection energy grid points is achieved by means of a one-mode approximation. Accurate results have been obtained with much coarser grids and significantly reduced computational time.

In the present paper we shall be concerned with the numerical analysis of the model introduced in [4], with the difference that we apply this model to describe the electron transport in a double-gate MOSFET device. A very fine discretization of the energy variable is thus not so necessary as for the RTD, so that only the WKB approximation shall be investigated. Moreover we shall use in this paper a finite element scheme rather than the finite volume scheme used in [4]. The resolution of the Schrödinger equation by standard finite elements (or finite volume schemes), requires a refined mesh size, due to the highly oscillating solutions for large electron energies E. The idea is to construct a Galerkin finite element method in which the approximating space is spanned by WKB basis functions. In contrast to the standard finite element methods, where the basis functions are picewise polynomial, the WKB basis functions are strongly oscillating, with a frequency close to that of the wave function. This WKB basis functions are determined asymptotically by the WKB approximation and are constituted of a smooth amplitude multiplied by an oscillating function of a phase, which is solution of the eiconal equation. The fact that the WKB basis functions incorporate *a priori* knowledge about the solution, avoids the restrictive choice of refined meshes. Accurate approximations are obtained with a large mesh size, independent on the energy E. The reduced number of unknowns naturally leads to a considerable gain in the simulation time.

The purpose of this paper is to prove consistency and stability of the method and to establish an error estimate in terms of the step size h and independent on the energy E and the rescaled Planck constant ε. The independence of the estimate on E and ε is the essential feature of this method. It allows the choice of a unique, relative coarse grid to achieve the same required accuracy for all possible wave-lengths $\lambda \sim \varepsilon/\sqrt{E}$.

Similar problems were investigated for the Helmholtz equation. In [10, 11], standard finite element methods, based on polynomial basis functions of order $p \geq 1$, are used for the resolution of the Helmholtz equation. Error estimates are derived for the 1D case, under the assumption $hk \leq 1$ and the constants involved in these estimates depend moreover on the term hk^2, with k the wave-vector and h the step size. This is rather restricitive from a numerical point of view. A more similar numerical asymptotic method, based also on the WKB approximation and applied to the Helmholtz equation is presented in [8]. The results obtained with this method are compared with the standard finite element method. However the mathematical and numerical analysis of the asymptotic method was not investigated.

This paper is organized as follows. Section 2 is devoted to the analysis of the continuous problem. In Section 3, the WKB basis functions are derived through the WKB asymptotics and the Galerkin finite element scheme is constructed. Finally, Section 4 is the main part of this paper and concerns the numerical analysis of the method. The consistency is investigated in Section 4.1 and the stability is treated in Section 4.2.

2 The continuous problem

2.1 Description of the model

The model problem we investigate in this paper is the one-dimensional stationary Schrödinger equation with open boundary conditions

$$\begin{cases} -\varepsilon^2 \psi_E''(x) + V(x)\psi_E(x) = E\psi_E(x)\,, \quad \text{in} \quad \text{(a,b)} \\ \psi_E'(a) + \mathbf{i}k_a\psi_E(a) = 2\mathbf{i}k_a \\ \psi_E'(b) - \mathbf{i}k_b\psi_E(b) = 0\,. \end{cases} \tag{2.1}$$

The equation describes the evolution of a wave-function ψ, penetrating the domain (a, b) from the left and being partially transmitted or reflected by the given electrostatic potential V. It is a quantum mechanical picture of an electron injected from the left into the device (a, b), with the injection-energy E. We shall consider in this paper the oscillating case, characterized by an injection energy E verifying $E - V(x) \geq \tau > 0$ in $[a, b]$, with τ a threshold value, fixed later on. The imposed boundary conditions are the so-called quantum transmitting boundary conditions (QTBM), introduced by Lent and Kirkner in [13] and enabeling the current flow through the boundaries. The wave-vector $k(x)$ and the de Broglie wave-length $\lambda(x)$ are given in terms of the energy by

$$k(x) := \frac{\sqrt{E - V(x)}}{\varepsilon} \quad ; \quad \lambda(x) = \frac{1}{k(x)} = \frac{\varepsilon}{\sqrt{E - V(x)}}\,. \tag{2.2}$$

The parameter ε stands for the rescaled Planck constant. We shall assume in this paper that ε is arbitrarly small, $0 < \varepsilon < 1$.
In the self-consistent case, the Schrödinger equation (2.1) is coupled with the Poisson equation, in order to compute the electrostatic potential. In this paper however, the potential is supposed to be fixed, as the coupling with Poisson does not change the subsequent analysis.

2.2 Existence, uniqueness and stability of a continuous solution

Let us start by analyzing equation (2.1) concerning the existence and uniqueness of solutions. The proof of the following theorem can be found in [2].

Theorem 2.1 (Existence + uniqueness)
Let $V \in L^\infty(a, b)$ and $0 < \varepsilon < 1$. Then, the equation (2.1) admits for all $E > V$ a unique solution $\psi_E \in W^{2,\infty}(a, b)$.

Estimates on this solution are given in the following

Theorem 2.2 (Boundedness)
Let $V \in W^{1,\infty}(a,b)$ and let $0 < \varepsilon < 1$ and E be arbitrary values with $E - V \geq \tau > 0$. Then the following estimates hold

$$||\psi_E||_{L^\infty(a,b)} \leq c \quad , \quad ||\frac{\varepsilon}{\sqrt{E-V}}\psi_E'||_{L^\infty(a,b)} \leq c\,, \tag{2.3}$$

with a constant $c > 0$ independent on ε and E.

Proof: The proof of this theorem relies on the Gronwall lemma. Let in the following $c_i > 0$ denote constants independent on ε and E. Multiplying the Schrödinger equation (2.1) by $\overline{\psi'}$, leads to

$$\varepsilon^2 \psi'' \overline{\psi'} + (E - V)\psi\overline{\psi'} = 0\,,$$

which can be rewritten by taking the real part in the form

$$\frac{\varepsilon^2}{2}\frac{d}{dx}|\psi'|^2 + \frac{E-V}{2}\frac{d}{dx}|\psi|^2 = 0\,.$$

Hence, using the fact that $V \in W^{1,\infty}(a,b)$ and $E - V \geq \tau > 0$, we deduce

$$\begin{aligned} \frac{d}{dx}\left[\varepsilon^2|\psi'|^2 + (E-V)|\psi|^2\right] &= -V'|\psi|^2 \leq c_1|\psi|^2 \\ &\leq c_2\left[\varepsilon^2|\psi'|^2 + (E-V)|\psi|^2\right]\,. \end{aligned}$$

Defining the auxiliary functions

$$G(x) := \varepsilon^2|\psi'|^2 + (E-V)|\psi|^2\,,$$

we have $G \geq 0$ and

$$\frac{d}{dx}G(x) \leq c_2 G(x)\,, \quad \text{in } [a,b]\,.$$

At this stage the Gronwall lemma yields

$$G(x) \leq G(a)e^{c_2(x-a)} \leq c_3 G(a)\,. \tag{2.4}$$

In order to deduce some estimates for ψ and ψ', it is thus necessary to estimate $\psi(a)$ and $\psi'(a)$. For this let us multiply the Schrödinger equation (2.1) by $\overline{\psi}$, integrate with respect to x, perform a partial integration and take the imaginary part. This yields

$$k_a|\psi(a)|^2 + k_b|\psi(b)|^2 = 2k_a\mathcal{R}e(\psi(a))\,,$$

implying

$$|\psi(a) - 1|^2 + \frac{k_b}{k_a}|\psi(b)|^2 = 1\,,$$

and thus $|\psi(a)| \leq 2$. The boundary condition $\psi'(a) + \mathbf{i}k_a\psi(a) = 2\mathbf{i}k_a$ yields immediately $|\psi'(a)| \leq 4k_a = 4\frac{\sqrt{E-V(a)}}{\varepsilon}$. Altogether we have $\frac{G(a)}{E-V(a)} \leq c_4$ and with (2.4) we get finally

$$\frac{\varepsilon^2}{E-V(x)}|\psi'(x)|^2 + |\psi(x)|^2 = \frac{G(x)}{E-V(x)} \leq c_5\,, \quad \forall x \in [a,b]\,,$$

with $c_5 > 0$ independent on ε and E. ∎

2.3 Variational formulation

In order to derive a discrete approximation scheme for the resolution of the Schrödinger equation, we need to introduce the variational formulation of problem (2.1). Hence, let us introduce the space $\mathcal{V}$ of test functions

$$\mathcal{V} := H^1(a,b)\,,$$

and define the following weighted norme in this space

$$||\theta||_{\mathcal{V}} := \left(||\theta||^2_{L^2} + \frac{\varepsilon^2}{E+||V||_\infty} ||\theta'||^2_{L^2} \right)^{1/2}\,, \quad \text{for} \quad \theta \in \mathcal{V}\,.$$

The variational formulation of (2.1) writes then: Find $\psi \in \mathcal{V}$, solution of

$$b(\psi,\theta) = L(\theta)\,, \quad \forall \theta \in \mathcal{V}\,, \tag{2.5}$$

with the sesquilinear form $b : \mathcal{V} \times \mathcal{V} \to \mathbb{C}$ given by

$$\begin{aligned} b(\psi,\theta) \;:=\; & \frac{\varepsilon^2}{E+||V||_\infty} \int_a^b \psi'(x)\overline{\theta}'(x)dx + \frac{1}{E+||V||_\infty} \int_a^b (V(x)-E)\psi(x)\overline{\theta}(x)dx - \\ & -\mathbf{i}k(a)\frac{\varepsilon^2}{E+||V||_\infty}\psi(a)\overline{\theta}(a) - \mathbf{i}k(b)\frac{\varepsilon^2}{E+||V||_\infty}\psi(b)\overline{\theta}(b)\,, \end{aligned}$$

and the antilinear form $L : \mathcal{V} \to \mathbb{C}$ defined as

$$L(\theta) := -2\mathbf{i}k(a)\frac{\varepsilon^2}{E+||V||_\infty}\overline{\theta}(a)\,.$$

This weak formulation is derived in standard manner, by multiplying (2.1) with the complex conjugate of a test function $\theta \in \mathcal{V}$ and integrating by parts. Notice that, the sesquilinear form b is continuous, but not hermitian and not coercive, the latter due to the negativity and non-boundedness of the term $V(x) - E$. Remark also, that Theorem 2.2 ensures the boundedness of the unique solution ψ_E in the $\mathcal{V}$-norm, uniformly in ε and E.
Hence we can pass to the discretization procedure.

3 The discrete problem

Starting from the variational formulation (2.5), a standard finite element method can be used to find an approximate solution of (2.1). In particular, the finite dimensional spaces $\mathcal{V}_h \subset \mathcal{V}$ could be chosen as consisting of continuous, picewise polynomial functions and the discrete method would write: Find $\psi_h \in \mathcal{V}_h$, solution of

$$b(\psi_h,\theta_h) = L(\theta_h)\,, \quad \forall \theta_h \in \mathcal{V}_h\,. \tag{3.1}$$

The disadvantage of this method is, that for high injection energies E a refined mesh size is required (10 node points per wavelength), to accurately approximate the highly oscillating solutions. This leads to high computational costs and simulation time. In order to overcome this limitation, one idea is to approximate the infinite dimensional space $\mathcal{V}$ by better adapted finite element spaces $\mathcal{V}_h$, which incorporate essential analytical properties of the solution of the differential equation. The hope is, that this spaces will be able to approximate better the exact solution than the spaces of picewise polynomial functions, and this independently on the wavevector k, avoiding thus the expensive refinement process.

3.1 A WKB finite element scheme

We shall expose now the main ideas how the finite dimensional spaces $\mathcal{V}_h$ are constructed, using the WKB approximation (see also [4]).
Let us partition the interval $[a, b]$ into $a = x_1 \leq x_2 \leq \cdots \leq x_N = b$ and denote the meshsize by $h_n := x_{n+1} - x_n$ and $h := max_n h_n$. The starting point is then the plane-wave Ansatz

$$\varphi(x) = e^{\mathbf{i} S_\varepsilon(x)/\varepsilon}, \tag{3.2}$$

where S_ε is the phase function, which may also be complex. We are searching for approximating solutions for the Schrödinger equation (2.1) in the form (3.2). Inserting thus this Ansatz in (2.1), leads to

$$-\mathbf{i}\varepsilon \left(\frac{d^2 S_\varepsilon}{dx^2} \right) + \left(\frac{dS_\varepsilon}{dx} \right)^2 + (V - E) = 0\,. \tag{3.3}$$

Approximating S_ε as a series of powers of ε

$$S_\varepsilon(x) = S_0(x) + \varepsilon S_1(x) + \frac{\varepsilon^2}{2} S_2(x) + \cdots,$$

substituting it into equation (3.3) and comparing the terms of the same order of ε, leads to a series of equations, to be solved to get S_0, S_1, S_2, ...

$$\begin{cases} (S_0')^2 + (V - E) = 0 \\ -\mathbf{i} S_0'' + 2 S_0' S_1' = 0 \\ -\mathbf{i} S_1'' + (S_1')^2 + S_0' S_2' = 0\,. \end{cases}$$

To stop the approximation at the first order term in ε, we will require, that $|\varepsilon S_2/2| \ll 1$, which writes

$$\left| \frac{\varepsilon V'(x)}{(E - V(x))^{3/2}} \right| \ll 1\,. \tag{3.4}$$

This criterion is the WKB validity condition. It signifies, that the changes of the potential energy within a de Broglie wavelength have to be small compared with the kinetic energy.
In order to applicate the WKB approximation, we have thus to avoid the turning points ($V(x) = E$). It is at this stage, that the threshold value $\tau > 0$ is chosen, and we shall assume in the following

Hypothesis A Let $0 < \varepsilon < 1$ be an arbitrary, real value and let the electrons be injected with an energy $E \in \mathbb{R}$ satisfying $E - V(x) \geq \tau$ for all $x \in [a, b]$, where $\tau > 0$ is chosen for a fixed potentiel V such that (3.4) is valid in $[a, b]$.

Then the WKB approximate solutions of the Schrödinger equation (2.1) in the interval $I_n = (x_n, x_{n+1})$ write

$$\varphi(x) = \frac{1}{\sqrt[4]{E - V(x)}} \left(A_n e^{\frac{\mathrm{i}}{\varepsilon} S_0(x)} + B_n e^{-\frac{\mathrm{i}}{\varepsilon} S_0(x)} \right), \tag{3.5}$$

with $S_0(x) := \int_{x_n}^{x} \sqrt{E - V(t)} dt$. These functions are the starting point for the derivation of the basis functions, being then used for the construction of the Galerkin finite element method. Straightforward calculations enable to rewrite the wavefunction (3.5) in each interval $I_n = (x_n, x_{n+1})$ as

$$\varphi(x) = w_n(x)\varphi^n + v_n(x)\varphi^{n+1} \quad , \quad \varphi^n := \varphi(x_n)\,, \tag{3.6}$$

with

$$\begin{aligned}
w_n(x) &:= \alpha_n(x) f_n(x) &;\quad v_n(x) &:= \beta_n(x) f_{n+1}(x)\,, \\
\alpha_n(x) &:= -\frac{sin\sigma_{n+1}(x)}{sin\gamma_n} &;\quad \beta_n(x) &:= \frac{sin\sigma_n(x)}{sin\gamma_n}\,, \\
\sigma_n(x) &:= \frac{1}{\varepsilon}\int_{x_n}^{x} \sqrt{E - V(t)} dt &;\quad \gamma_n &:= \frac{1}{\varepsilon}\int_{x_n}^{x_{n+1}} \sqrt{E - V(t)} dt\,,
\end{aligned} \tag{3.7}$$

and the amplitude factors

$$f_n(x) := \sqrt[4]{\frac{E - V(x_n)}{E - V(x)}}\,. \tag{3.8}$$

The functions α_n^j and β_n^j are the so-called WKB basis functions. They oscillate with a frequency close to that of the unknown wave function and actually permit solving the problem on coarser grids. In the limit $h \ll \lambda$, these WKB basis functions reduce to usual linear interpolation functions.
To avoid division by zero, let the following Hypothesis be verified in the sequel.

Hypothesis B Let $\gamma > 0$ be a fixed constant and assume that the following statement holds for all n

$$\left| \frac{1}{\varepsilon} \int_{x_n}^{x_{n+1}} \sqrt{E - V(t)} dt - k\pi \right| \geq \gamma\,, \quad \forall k \in \mathbb{N} \backslash \{0\}\,,$$

such that we can estimate

$$|\sin \gamma_n| \geq c_\gamma\,, \quad \forall \gamma_n \text{ far from zero}\,,$$

with $c_\gamma > 0$ a constant independent on ε, E and h.

Hence possessing in each I_n basis functions, asymptotically derived from the WKB Ansatz, we introduce an appropriate finite dimensional space $\mathcal{V}_h$ as

$$\mathcal{V}_h := \left\{ \theta_h \in \mathcal{V} \ \ / \ \ \theta_h(x) = \sum_{n=1}^{N} z_n \zeta_n(x), \quad z_n \in \mathbb{C} \right\}, \tag{3.9}$$

where ζ_n are the so-called "WKB hat-functions"

$$\zeta_n(x) := \begin{cases} v_{n-1}(x), & \text{in} \quad [x_{n-1}, x_n] \\ w_n(x), & \text{in} \quad [x_n, x_{n+1}]\,. \end{cases} \tag{3.10}$$

The WKB finite element method states finally: Find $\psi_h \in \mathcal{V}_h$, solution of

$$b(\psi_h, \theta_h) = L(\theta_h), \quad \forall \theta_h \in \mathcal{V}_h\,, \tag{3.11}$$

with the linear forms b and L given in Section 2.3. The subscript h refers to the discretization of (a, b) and emphasizes the dependence of the discrete solution on the meshsize.

In Figure 1 we illustrate a "hat-function", constructed with the WKB basis functions and, as comparison, a standard linear hat-function.

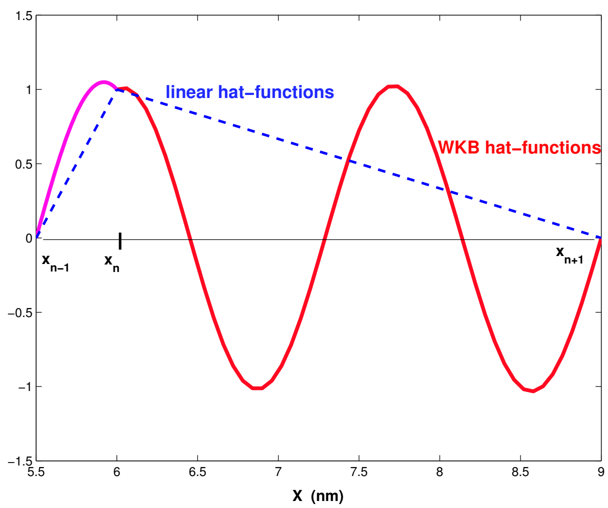

Figure 1: A WKB hat-function and a standard linear hat-function, on an irregular grid.

Remark 3.1 *The WKB hat functions ζ_n are solutions of the following equation*

$$-\varepsilon^2 \frac{d^2}{dx^2}\zeta_n + \varepsilon^2 \left(\frac{1}{4}\frac{V''(x)}{E - V(x)} + \frac{5}{16}\frac{(V'(x))^2}{(E - V(x))^2} \right) \zeta_n + (V(x) - E)\zeta_n = 0\,. \tag{3.12}$$

For notational simplicity, we shall use in the sequel the abbreviation

$$W(x) := \frac{1}{4}\frac{V''(x)}{E - V(x)} + \frac{5}{16}\frac{(V'(x))^2}{(E - V(x))^2}\,. \tag{3.13}$$

Let us now proceed to an $\mathcal{V}$-estimate of the WKB hat-functions ζ_n.

Lemma 3.2 *Let $V \in W^{1,\infty}(a,b)$ and let Hypothesis A and B be satisfied. Then the WKB hat-functions satisfy for each $n \in \{1, \cdots, N\}$ the estimates*

$$||\zeta_n||_{L^\infty(I_{n-1}\cup I_n)} \le c \quad ; \quad ||\zeta_n'||_{L^\infty(I_{n-1}\cup I_n)} \le c \left(\frac{h}{h_{n-1}h_n} + \frac{1}{\lambda_n} \right) , \tag{3.14}$$

and hence

$$||\zeta_n||_{\mathcal{V}} \le c\sqrt{h} \frac{\varepsilon}{\sqrt{E + ||V||_\infty}} \left(\frac{h}{h_{n-1}h_n} + \frac{1}{\lambda_n} \right) , \tag{3.15}$$

where $\lambda_n := \lambda(x_n)$ and the constants $c > 0$ are independent on ε, E and h.

Proof: We start by rewriting $\zeta_n(x)$ and $\zeta_n'(x)$ in their corresponding support intervals (x_{n-1}, x_{n+1}).

$$\zeta_n(x) := \begin{cases} \dfrac{(E-V_n)^{1/4}}{(E-V(x))^{1/4}} \dfrac{sin\left(\dfrac{1}{\varepsilon}\displaystyle\int_{x_{n-1}}^{x} \sqrt{E-V(t)}dt\right)}{sin\left(\dfrac{1}{\varepsilon}\displaystyle\int_{x_{n-1}}^{x_n} \sqrt{E-V(t)}dt\right)}, & \text{in} \quad [x_{n-1}, x_n] \\ -\dfrac{(E-V_n)^{1/4}}{(E-V(x))^{1/4}} \dfrac{sin\left(\dfrac{1}{\varepsilon}\displaystyle\int_{x_{n+1}}^{x} \sqrt{E-V(t)}dt\right)}{sin\left(\dfrac{1}{\varepsilon}\displaystyle\int_{x_n}^{x_{n+1}} \sqrt{E-V(t)}dt\right)}, & \text{in} \quad [x_n, x_{n+1}] , \end{cases}$$

$$\zeta_n'(x) := \begin{cases} \dfrac{1}{4} \dfrac{(E-V_n)^{1/4} V'(x)}{(E-V(x))^{5/4}} \dfrac{sin\,(\sigma_{n-1}(x))}{sin\,(\gamma_{n-1})} + \\ \qquad + \dfrac{(E-V_n)^{1/4}}{(E-V(x))^{1/4}} \dfrac{cos\,(\sigma_{n-1}(x))}{sin\,(\gamma_{n-1})} \dfrac{1}{\varepsilon} (E-V(x))^{1/2}, & \text{in} \quad (x_{n-1}, x_n), \\ -\dfrac{1}{4} \dfrac{(E-V_n)^{1/4} V'(x)}{(E-V(x))^{5/4}} \dfrac{sin\,(\sigma_{n+1}(x))}{sin\,(\gamma_n)} - \\ \qquad - \dfrac{(E-V_n)^{1/4}}{(E-V(x))^{1/4}} \dfrac{cos\,(\sigma_{n+1}(x))}{sin\,(\gamma_n)} \dfrac{1}{\varepsilon} (E-V(x))^{1/2}, & \text{in} \quad (x_n, x_{n+1}) . \end{cases}$$

Two cases have now to be considered separately.

Case I: Let $h_n \le \frac{1}{2}\lambda(x)$ in I_n.
This case corresponds to a meshsize smaller than the de Broglie wavelength and includes also the particular case $h_n \ll \lambda$ of linear interpolation functions. The characteristic feature of this case is that the phase function σ_{n+1} is close to zero, enabeling thus the following expansion for $x \in I_n$

$$sin\,(\sigma_{n+1}(x)) = \sigma_{n+1}(x) \left(1 - \frac{\sigma_{n+1}^2(x)}{6} cos(\xi) \right) , \quad \text{with} \quad \xi \in (0, \sigma_{n+1}(x)) ,$$

where due to the fact that $h_n/\lambda \leq 1/2$, we have

$$\left|\frac{\sigma_{n+1}^2(x)}{6} cos(\xi)\right| \leq \frac{1}{24}\,.$$

Hypothesis A as well as the assumption that V belongs to $W^{1,\infty}(a,b)$, enables us to write by a simple Taylor expansion

$$\left|\frac{E-V(y)}{E-V(x)}-1\right| \leq c|y-x|\,,$$

with $c>0$ independent on E, implying thus immediately the estimates

$$||\zeta_n||_{L^\infty(I_n)} \leq c \quad ; \quad ||\zeta_n'||_{L^\infty(I_n)} \leq c\frac{1}{h_n}\,,$$

with $c>0$ independent on ε and E. Analogously we would get for the neighbouring interval I_{n-1}, in the case $h_{n-1} \leq \frac{1}{2}\lambda(x)$, the estimates

$$||\zeta_n||_{L^\infty(I_{n-1})} \leq c \quad ; \quad ||\zeta_n'||_{L^\infty(I_{n-1})} \leq c\frac{1}{h_{n-1}}\,.$$

Case II: Let $h_n > \frac{1}{2}\lambda(x_0)$ for some $x_0 \in I_n$. Then there exists a constant $0 < c_0 \leq 1/2$, independent on n, ε and E, such that $h_n > c_0\lambda(x)$ in I_n. Indeed, expanding λ around x_0 and using the validity conditon (3.4), yields $c_0 = 2/5$.
In contrast to the previous case, this case represents the situation where the stepsize is larger than the de Broglie wavelength and where the WKB oscillating basis functions start to be useful. Being far from $\gamma_n = k\pi\ \forall k \in \mathbb{N}$, we have the estimate

$$c_\gamma \leq |sin(\gamma_n)| \leq 1\,,$$

and deduce thus

$$||\zeta_n||_{L^\infty(I_n)} \leq c \quad ; \quad ||\zeta_n'||_{L^\infty(I_n)} \leq c\frac{1}{\lambda_n}\,,$$

with $c>0$ independent on ε and E. The same estimates hold for the neighbouring interval I_{n-1}.
Bringing together these results yields the $\mathcal{V}$-estimate for the WKB basis function ζ_n.

∎

3.2 Existence, uniqueness of a discrete solution

The question to be posed now is, wether the discrete problem (3.11) has a solution $\psi_h \in \mathcal{V}_h$ and if this solution is unique.

Theorem 3.3 (Existence + uniqueness result)
Let $V \in L^\infty(a,b)$. Then assuming Hypothesis A and B, the discrete problem (3.11) admits a unique solution $\psi_h \in \mathcal{V}_h$ for every $0 < h < h_*$, with $0 < h_* < 1$ a value independent on ε and E.

Proof: We seek for a solution belonging to $\mathcal{V}_h$, thus of the form $\psi_h(x) = \sum_{n=1}^N z_n \zeta_n(x)$. Substituting this expression in (3.11) and choosing as test functions the basis functions $\zeta_i(x)$, leads to a linear system to be solved to determine the unknows z_n

$$\begin{pmatrix} b(\zeta_1,\zeta_1) & b(\zeta_2,\zeta_1) & \cdots & b(\zeta_N,\zeta_1) \\ b(\zeta_1,\zeta_2) & b(\zeta_2,\zeta_2) & \cdots & b(\zeta_N,\zeta_2) \\ \vdots & \vdots & & \vdots \\ b(\zeta_1,\zeta_N) & b(\zeta_2,\zeta_N) & \cdots & b(\zeta_N,\zeta_N) \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_N \end{pmatrix} = \begin{pmatrix} L(\zeta_1) \\ L(\zeta_2) \\ \vdots \\ L(\zeta_N) \end{pmatrix}. \tag{3.16}$$

Let us denote in the sequel by M the matrix of this linear system. M is a tridiagonal matrix due to the fact that the supports of the basis functions ζ_i cover only the two intervals I_{i-1} and I_i. To prove that this system has a unique solution, we have to show, that the corresponding homogenous system $Mz = 0$ admits as unique solution $z \equiv 0$. The homogenous system corresponds to $b(\psi_h, \zeta_i) = 0\ \forall i$, hence $b(\psi_h, \psi_h) = 0$. Taking the imaginary part of this last equation yields $\psi_h(a) = \psi_h(b) = 0$, which means $z_1 = z_N = 0$. The next lemma will show that $b(\zeta_{i+1}, \zeta_i) \neq 0\ \forall i$, which permits to conclude immediately that $z_i = 0\ \forall i$, by solving the homogenous system step by step. This implies that M is invertible and as such that the system (3.16) is uniquely solvable. Thus to finish our proof we shall analyze in the following lemma the asymptotic behaviour of the terms $b(\zeta_{i+1}, \zeta_i)$. ∎

Lemma 3.4 *Let $V \in W^{2,\infty}(a,b)$. Assuming Hypothesis A and B, there exists a value $0 < h_* < 1$, independent on ε and E, so that for every discretization with $0 < h < h_*$, the terms $b(\zeta_{n+1}, \zeta_n)$ and $b(\zeta_n, \zeta_n)$ verify $\forall n \in \{1, \cdots, N\}$ the estimates*

$$c_1 \frac{\varepsilon^2}{E + ||V||_\infty} \left(\frac{1}{h_n} + \frac{1}{\lambda_n} \right) \ \leq\ |b(\zeta_{n+1}, \zeta_n)| \ \leq\ c_2 \frac{\varepsilon^2}{E + ||V||_\infty} \left(\frac{1}{h_n} + \frac{1}{\lambda_n} \right),$$

$$0 \ \leq\ |b(\zeta_n, \zeta_n)| \ \leq\ c_3 \frac{\varepsilon^2}{E + ||V||_\infty} \left(\frac{h}{h_{n-1} h_n} + \frac{1}{\lambda_n} \right),$$

with positive constants c_1, c_2, c_3 independent on the parameters ε, E and h. Remark that $b(\zeta_{n+1}, \zeta_n) = b(\zeta_n, \zeta_{n+1})$. Moreover the following asymptotic behaviours hold for $n = 2, \ldots, N-1$

$$\begin{aligned}
\frac{b(\zeta_N,\zeta_N)}{b(\zeta_{N-1},\zeta_N)} &= -\left[e^{-\mathrm{i}\gamma_{N-1}} + \frac{\varepsilon \sin\gamma_{N-1}}{\sqrt{E - V_N}} \left(\frac{1}{4} \frac{V'(x_N)}{E - V_N} - \int_{x_{N-1}}^{x_N} W(x) |\zeta_N|^2 dx \right) \right] (1 + \mathcal{O}(h)), \\
\frac{b(\zeta_n,\zeta_n)}{b(\zeta_{n-1},\zeta_n)} &= -\left[\frac{\sin(\gamma_n + \gamma_{n-1})}{\sin\gamma_n} - \frac{\varepsilon \sin\gamma_{n-1}}{\sqrt{E - V_n}} \int_{x_{n-1}}^{x_{n+1}} W(x) |\zeta_n|^2 dx \right] (1 + \mathcal{O}(h)), \\
\frac{b(\zeta_{n+1},\zeta_n)}{b(\zeta_{n-1},\zeta_n)} &= \left[\frac{\sin\gamma_{n-1}}{\sin\gamma_n} + \frac{\varepsilon \sin\gamma_{n-1}}{\sqrt{E - V_n}} \frac{(E - V_n)^{1/4}}{(E - V_{n+1})^{1/4}} \int_{x_n}^{x_{n+1}} W(x) \zeta_{n+1} \zeta_n dx \right] (1 + \mathcal{O}(h)), \\
&= \frac{\sin\gamma_{n-1}}{\sin\gamma_n} (1 + \mathcal{O}(h))^2,
\end{aligned} \tag{3.17}$$

with W given by (3.13). The notation $\mathcal{O}(h)$ stands for terms g of the order of the meshsize h, more precisely satisfying $|g| \leq ch$ with a constant $c > 0$ independent on ε, E, h and n.

Proof: Performing a partial integration and using the fact that ζ_n are solutions of the equation (3.12), we can write the term $b(\zeta_{n+1}, \zeta_n)$ under the form

$$\begin{aligned} b(\zeta_{n+1}, \zeta_n) &= \frac{\varepsilon^2}{E + ||V||_\infty} \int_{x_n}^{x_{n+1}} \zeta_{n+1}' \zeta_n' dx + \frac{1}{E + ||V||_\infty} \int_{x_n}^{x_{n+1}} (V(x) - E) \zeta_{n+1} \zeta_n dx \\ &= \frac{-\varepsilon^2}{E + ||V||_\infty} \left[\zeta_{n+1}'(x_n) + \int_{x_n}^{x_{n+1}} \left(\frac{1}{4} \frac{V''(x)}{E - V} + \frac{5}{16} \frac{(V'(x))^2}{(E - V)^2} \right) \zeta_{n+1} \zeta_n dx \right], \end{aligned} \tag{3.18}$$

where

$$\zeta_{n+1}'(x_n) = \frac{(E - V_{n+1})^{1/4}}{(E - V_n)^{1/4}} \frac{\sqrt{E - V_n}}{\varepsilon} \cdot \frac{1}{\sin \gamma_n}.$$

Similarly

$$b(\zeta_n, \zeta_n) = \frac{-\varepsilon^2}{E + ||V||_\infty} \left[\zeta_n'(x_n^+) - \zeta_n'(x_n^-) + \int_{x_{n-1}}^{x_{n+1}} \left(\frac{1}{4} \frac{V''(x)}{E - V} + \frac{5}{16} \frac{(V'(x))^2}{(E - V)^2} \right) |\zeta_n|^2 dx \right], \tag{3.19}$$

with

$$\zeta_n'(x_n^+) - \zeta_n'(x_n^-) = -\frac{\sqrt{E - V_n}}{\varepsilon} \left(\frac{\cos \gamma_n}{\sin \gamma_n} + \frac{\cos \gamma_{n-1}}{\sin \gamma_{n-1}} \right),$$

and

$$b(\zeta_N, \zeta_N) = \frac{-\varepsilon^2}{E + ||V||_\infty} \left[-\zeta_N'(x_N^-) + \mathbf{i} k_b + \int_{x_{N-1}}^{x_N} \left(\frac{1}{4} \frac{V''(x)}{E - V} + \frac{5}{16} \frac{(V'(x))^2}{(E - V)^2} \right) |\zeta_N|^2 dx \right], \tag{3.20}$$

with

$$\zeta_N'(x_N^-) = \frac{1}{4} \frac{V'(x_N)}{E - V_N} + \frac{\sqrt{E - V_N}}{\varepsilon} \frac{\cos \gamma_{N-1}}{\sin \gamma_{N-1}}.$$

We proceed now in two steps, corresponding to a meshsize h_n smaller respectively larger than the de Broglie wavelength, as done in the proof of Lemma 3.2.

Case I: Let $h_n \le \frac{1}{2} \lambda(x)$ in I_n.
On one hand, we have with Lemma 3.2 immediately

$$|b(\zeta_{n+1}, \zeta_n)| \le c \frac{\varepsilon^2}{E + ||V||_\infty} \left(\frac{1}{h_n} + c h_n \right) \le c \frac{\varepsilon^2}{E + ||V||_\infty} \frac{1}{h_n}.$$

To get the other estimate, we shall use in this case that $|sin(\sigma)| \le |\sigma|$. There exists a value $0 < h_* < 1$, sufficiently small, but independent on ε and E, such that we have for meshsizes $h < h_*$

$$|\zeta_{n+1}'(x_n)| \ge c \frac{1}{h_n},$$

implying, by adapting h_*, the following estimate with $c > 0$ independent on ε and E

$$|b(\zeta_{n+1}, \zeta_n)| \ge c \frac{\varepsilon^2}{E + ||V||_\infty} \left(\frac{1}{h_n} - c h_n \right) \ge c \frac{\varepsilon^2}{E + ||V||_\infty} \frac{1}{h_n}.$$

Case II: Let $h_n > c_0 \lambda(x)$ in I_n.
A direct conclusion of Lemma 3.2 and the estimate $c_\gamma \le |\sin \gamma_n|$ is

$$|b(\zeta_{n+1},\zeta_n)| \le c \frac{\varepsilon^2}{E+||V||_\infty}\left(\frac{1}{\lambda_n}+ch_n\right) \le c\frac{\varepsilon^2}{E+||V||_\infty}\frac{1}{\lambda_n}\,.$$

The minoration is deduced from the fact, that $|sin(\sigma)| \le 1$, leading for $h < h_*$ with $0 < h_* < 1$ small enough but independent on ε and E, to

$$|\zeta'_{n+1}(x_n)| \ge c\frac{1}{\lambda_n}\,,$$

and hence

$$|b(\zeta_{n+1},\zeta_n)| \ge c \frac{\varepsilon^2}{E+||V||_\infty}\left(\frac{1}{\lambda_n}-ch_n\right) \ge c\frac{\varepsilon^2}{E+||V||_\infty}\frac{1}{\lambda_n}\,.$$

Combining these estimates, yields the desired result for the term $b(\zeta_{n+1},\zeta_n)$. Similar arguments enable to get the estimate for the term $b(\zeta_n,\zeta_n)$. Due to the fact, that the difference $|\zeta'_n(x_n^+)-\zeta'_n(x_n^-)|$ can not be minorated in the case $h_n > c_0\lambda(x)$, we have not the minoration estimate as for the term $b(\zeta_{n+1},\zeta_n)$.
The expressions (3.17) are deduced immediately from (3.18)-(3.20). It is important for the subsequent analysis to show that the terms denoted by $\mathcal{O}(h)$ are of the order of the meshsize h and this independently on the parameters ε and E. To this aim, let us detail here the derivation of the asymptotic behaviour of one of the terms (3.17). We have for $n \ne 1$, $n \ne N$

$$\begin{aligned}
\frac{b(\zeta_n,\zeta_n)}{b(\zeta_{n-1},\zeta_n)} &= -\left[\frac{\sqrt{E-V_n}}{\varepsilon}\frac{\sin(\gamma_n+\gamma_{n-1})}{\sin\gamma_{n-1}\sin\gamma_n} - \int_{x_{n-1}}^{x_{n+1}} W(x)|\zeta_n|^2dx\right]\cdot \\
&\qquad \cdot\left[\frac{(E-V_n)^{1/4}}{(E-V_{n-1})^{1/4}}\frac{\sqrt{E-V_{n-1}}}{\varepsilon}\frac{1}{\sin\gamma_{n-1}} + \int_{x_{n-1}}^{x_n} W(x)\zeta_n\zeta_{n-1}dx\right]^{-1} \\
&= -\left[\frac{\sin(\gamma_n+\gamma_{n-1})}{\sin\gamma_n} - \frac{\varepsilon\sin\gamma_{n-1}}{\sqrt{E-V_n}}\int_{x_{n-1}}^{x_{n+1}} W(x)|\zeta_n|^2dx\right]Q_n\,,
\end{aligned}$$

with

$$Q_n := \left[\frac{(E-V_n)^{1/4}}{(E-V_{n-1})^{1/4}}\frac{\sqrt{E-V_{n-1}}}{\sqrt{E-V_n}} + \frac{\varepsilon\sin\gamma_{n-1}}{\sqrt{E-V_n}}\int_{x_{n-1}}^{x_n} W(x)\zeta_n\zeta_{n-1}dx\right]^{-1}\,.$$

Due to Hypothesis A, the fact that the hat-functions ζ_n are uniformly bounded in $L^\infty(a,b)$ and that $V \in W^{2,\infty}(a,b)$, we can easily show for $h < h_*$, with a readjusted $0 < h_* < 1$ but still independent on ε and E, that

$$|Q_n - 1| \le ch\,, \quad \text{with } c>0 \quad \text{independent on} \quad \varepsilon,\ E,\ \text{and } N\,.$$

Analogously we obtain the other asymptotic behaviours. ∎

Another important question is wether the discrete solution $\psi_h \in \mathcal{V}$ is bounded in the $\mathcal{V}$-norm, and this independently on the parameters ε, E and on the meshsize h. This will be the aim of the next theorem.

Theorem 3.5 (Boundedness result)
Let $h < h_*$ and $\psi_h \in \mathcal{V}_h$ be the unique solution of the problem (3.11). Then we have the $\mathcal{V}$-estimate

$$||\psi_h||_{\mathcal{V}} \le c\,, \quad \textit{with } c > 0 \textit{ independent on } \varepsilon,\ E \textit{ and } h.$$

Proof: From now on, we shall denote by $c > 0$ a constant independent on ε, E and h. Writing the discrete solution $\psi_h \in \mathcal{V}_h$ of problem (3.11) in terms of the basis functions ζ_n as follows

$$\psi_h(x) = \sum_{n=1}^{N} z_n \zeta_n(x)\,, \tag{3.21}$$

we observe, that it suffices to show that the coefficients z_n satisfy $|z_n| \le c\ \forall n$, to get the boundedness of ψ_h in the $\mathcal{V}$-norm. Indeed, $|z_n| \le c\ \forall n$ implies with Lemma 3.2

$$\begin{aligned}\int_a^b |\psi_h(x)|^2 dx &= \sum_{n=1}^{N} \left(z_n \overline{z_{n-1}} \int_{x_{n-1}}^{x_n} \zeta_n \zeta_{n-1} dx + |z_n|^2 \int_{x_{n-1}}^{x_{n+1}} |\zeta_n|^2 dx + z_n \overline{z_{n+1}} \int_{x_n}^{x_{n+1}} \zeta_n \zeta_{n+1} dx \right) \\ &\le \ c\,.\end{aligned}$$

Moreover, taking the real part of the equation $b(\psi_h, \psi_h) = L(\psi_h)$, we can estimate the derivative term as

$$\frac{\varepsilon^2}{E + ||V||_\infty} \int_a^b |\psi_h'(x)|^2 dx \le \int_a^b |\psi_h(x)|^2 dx + 2k_a \frac{\varepsilon^2}{E + ||V||_\infty} |\psi_h(a)| \le c\,,$$

which implies the desired result.

Let us thus prove, that the coefficients z_n of the decomposition (3.21) are bounded independently on ε, E and h. These coefficients are solution of the linear system (3.16), with M a tridiagonal matrix and $L(\zeta_l) = 0$, for $l = 2, \cdots, N$. Taking the imaginary part of the equation $b(\psi_h, \psi_h) = L(\psi_h)$, we obtain

$$k_a \frac{\varepsilon^2}{E + ||V||_\infty} |z_1|^2 + k_b \frac{\varepsilon^2}{E + ||V||_\infty} |z_N|^2 = 2k_a \frac{\varepsilon^2}{E + ||V||_\infty} \mathcal{R}e(z_1)\,,$$

which yields the boundedness of z_1 and z_N, in particular

$$|z_1| \le 2 \quad ; \quad |z_N| \le \sqrt{\frac{k_a}{k_b}} \le c\,, \quad \text{with } c > 0 \quad \text{independent on} \quad \varepsilon,\, E\,.$$

Starting from the last line of the linear system (3.16), we are now able to show, step by step, the boundedness of all coefficients. Indeed, with expressions (3.17), we can write

$$z_{N-1} = -\frac{b(\zeta_N, \zeta_N)}{b(\zeta_{N-1}, \zeta_N)} z_N = (\eta_{N-1} + \kappa_{N-1} \sin \gamma_{N-1})(1 + \mathcal{O}(h)) z_N\,,$$

with

$$\eta_{N-1} = e^{-\mathbf{i}\gamma_{N-1}} \quad ; \quad \kappa_{N-1} = \frac{\varepsilon}{\sqrt{E - V_N}} \left(\frac{1}{4} \frac{V'(x_N)}{E - V_N} - \int_{x_{N-1}}^{x_N} W(x) |\zeta_N|^2 dx \right)\,. \tag{3.22}$$

Straightforward calculations yield by induction the following expressions for z_{N-i} in terms of z_N and for $i = 2, \ldots, N-2$:

$$\begin{aligned} z_{N-i} &= -\frac{b(\zeta_{N-i+1}, \zeta_{N-i+1})}{b(\zeta_{N-i}, \zeta_{N-i+1})} z_{N-i+1} - \frac{b(\zeta_{N-i+2}, \zeta_{N-i+1})}{b(\zeta_{N-i}, \zeta_{N-i+1})} z_{N-i+2} \\ &= (\eta_{N-i} + \kappa_{N-1} \sin(\gamma_{N-1} + \ldots + \gamma_{N-i}) + \ldots + \kappa_{N-i} \sin(\gamma_{N-i}))(1 + \mathcal{O}(h))^i z_N \,, \end{aligned}$$

with

$$\eta_{N-i} = e^{-\mathbf{i}(\gamma_{N-1} + \ldots + \gamma_{N-i})} \,, \tag{3.23}$$

and

$$\begin{aligned} \kappa_{N-j} &= -\left(\eta_{N-j+1} + \kappa_{N-1} \sin(\gamma_{N-1} + \ldots + \gamma_{N-j+1}) + \ldots + \kappa_{N-j+1} \sin(\gamma_{N-j+1})\right) \\ &\quad \frac{\varepsilon}{\sqrt{E - V_{N-j+1}}} \int_{x_{N-j}}^{x_{N-j+2}} W(x) |\zeta_{N-j+1}|^2 dx \,, \quad j = 2, \ldots, N-2 \,. \end{aligned} \tag{3.24}$$

This can be simply verified by observing that

$$\sin(\mu + \nu) e^{-\mathbf{i}(\rho + \mu)} - \sin(\nu) e^{-\mathbf{i}\rho} = \sin(\mu) e^{-\mathbf{i}(\rho + \mu + \nu)} \,, \quad \forall \, \mu, \nu, \rho \in \mathbb{R} \,.$$

In order to prove the boundedness of the coefficients z_{N-i} we have thus to estimate the terms κ_{N-j}. Observe that $|\eta_{N-j}| = 1$, $\forall j = 1, \ldots, N-2$. Setting $\kappa := |\kappa_{N-1}| \le c$, we get by simple induction arguments

$$|\kappa_{N-j}| \le ch(1 + \kappa)(1 + ch)^{j-2} \,, \quad j = 2, \ldots, N-2 \,, \tag{3.25}$$

with a constant $c > 0$ independent on ε, E and h. Thus we deduce

$$\begin{aligned} |z_{N-i}| &\le \left(1 + \kappa + \sum_{j=2}^{i} ch(1 + \kappa)(1 + ch)^{j-2}\right)(1 + ch)^i |z_N| \\ &= (1 + \kappa)(1 + ch)^{2i-1} |z_N| \,, \quad i = 1, \ldots, N-2 \,, \end{aligned}$$

implying the boundedness of the coefficients z_n independently on ε, E and the meshsize $h < h_*$. ∎

4 Convergence of the numerical scheme

This section is devoted to the convergence study of the just constructed numerical scheme, in particular to the derivation of error estimates. Let in the following ψ be the exact solution of (2.1), ψ_h the discrete one, solution of (3.11), and let $\Pi_h^{\varepsilon,E} \psi \in \mathcal{V}_h$ be the interpolant of ψ. The projection operator is defined by

$$\Pi_h^{\varepsilon,E} : \mathcal{V} \to \mathcal{V}_h \,, \quad \text{with} \quad \Pi_h^{\varepsilon,E} \varphi(x) = \sum_{i=1}^{N} \varphi(x_i) \zeta_i(x) \,, \quad \forall \varphi \in \mathcal{V} \,. \tag{4.1}$$

To ensure that the discrete solution ψ_h converge in the $\mathcal{V}$-norm towards the exact solution ψ, as the stepwidth h tends to zero, we have to show an estimate on the error $e_h := \psi - \psi_h$ in terms of h. The investigation of this error term is the subject of the subsequent analysis. Let us state the main theorem of this paper.

Theorem 4.1 (Convergence)
Let $V \in W^{2,\infty}(a,b)$. Under Hypothesis A and B, the WKB finite element error between the exact solution ψ and the discrete one ψ_h, satisfies the estimate

$$||\psi - \psi_h||_{\mathcal{V}} \leq ch \left(h + \frac{\varepsilon}{\sqrt{E + ||V||_\infty}} \right) , \tag{4.2}$$

with $h := max_n h_n$ satisfying $h < h_*$, where h_* is independent on ε, E, and with $c > 0$ a constant independent on ε, E and h.

We emphasize that the independence of this estimate on ε and E signifies that the stepsize h has not to be adjusted to the wavelength λ. This is the essential advantage to the standard finite element schemes. A unique coarse grid, consisting of multi-wavelength size elements, can be chosen to approximate the solution of the Schrödinger equation with a desired accuracy, independently on the electron injection energy E.
The proof of this theorem consists in two steps, studied in the following two sections. Obviously

$$||e_h||_{\mathcal{V}} \leq ||\psi - \Pi_h^{\varepsilon,E}\psi||_{\mathcal{V}} + ||\Pi_h^{\varepsilon,E}\psi - \psi_h||_{\mathcal{V}} \,,$$

and each of these terms shall now be analyzed separately.

4.1 Consistency

The goal of this section is to estimate the interpolation error $e_{1,h}(x) := \psi(x) - \Pi_h^{\varepsilon,E}\psi(x)$ in the $\mathcal{V}$-norm. For notational simplicity, we shall often omit the index ε and E of the interpolant.

Theorem 4.2 (Interpolation error)
Let $V \in W^{2,\infty}(a,b)$. Under the Hypothesis A and B, the interpolation error of the exact solution ψ, in the $\mathcal{V}$-norm, is estimated as follows

$$||\psi - \Pi_h^{\varepsilon,E}\psi||_{\mathcal{V}} \leq ch \left(h + \frac{\varepsilon}{\sqrt{E + ||V||_\infty}} \right) ||\psi||_{L^2(a,b)} \,, \tag{4.3}$$

where $\Pi_h^{\varepsilon,E}$ is the interpolation operator defined in (4.1), $h := max_n h_n$, $h < h_*$ with h_* independent on ε, E, and where $c > 0$ is a constant independent on ε, E and h. In particular we have

$$||\psi - \Pi_h^{\varepsilon,E}\psi||_{L^\infty(a,b)} \leq ch^2 ||\psi||_{L^\infty(a,b)} \quad ; \quad ||(\psi - \Pi_h^{\varepsilon,E}\psi)'||_{L^\infty(a,b)} \leq ch||\psi||_{L^\infty(a,b)} \,.$$

Proof: We shall prove the estimate picewise, in each $I_n = (x_n, x_{n+1})$, the stated result follows then by summing over n. Recall that

$$\Pi_h\psi(x) = w_n(x)\psi^n + v_n(x)\psi^{n+1} \,,$$

with w_n and v_n given by the formulae (3.7). The boundary conditions, these functions satisfy, are

$$w_n(x_n) = 1 \,, \quad w_n(x_{n+1}) = 0 \quad ; \quad v_n(x_n) = 0 \,, \quad v_n(x_{n+1}) = 1 \,.$$

Note moreover, that w_n and v_n are exact solutions of a slightly changed Schrödinger equation of the type

$$\mathcal{A}_{\varepsilon,E}\theta = 0\,,$$

with the operator

$$\mathcal{A}_{\varepsilon,E} := -\varepsilon^2 \frac{d^2}{dx^2} + \varepsilon^2 \left(\frac{1}{4} \frac{V''(x)}{E - V(x)} + \frac{5}{16} \frac{(V'(x))^2}{(E - V(x))^2} \right) + (V(x) - E)\,. \tag{4.4}$$

The exact solution ψ of (2.1) satisfies the equation

$$\mathcal{A}_{\varepsilon,E}\psi = \varepsilon^2 r(x)\,,$$

with a rest term r, given by

$$r(x) = \left(\frac{1}{4} \frac{V''(x)}{E - V(x)} + \frac{5}{16} \frac{(V'(x))^2}{(E - V(x))^2} \right) \psi.$$

Thus, the interpolation error function $e_{1,h}(x) = \psi(x) - \Pi_h \psi(x)$, is solution of the following system

$$\begin{cases} \mathcal{A}_{\varepsilon,E} e_{1,h} = \varepsilon^2 r\,, & in \quad I_n \\ e_{1,h}(x_n) = e_{1,h}(x_{n+1}) = 0\,. \end{cases} \tag{4.5}$$

The functions w_n and v_n are linear independent solutions of the corresponding homogenous equation. Applying thus the "variation of constants" method, starting from the Ansatz

$$e_{1,h}(x) = c_1(x) w_n(x) + c_2(x) v_n(x)\,,$$

we deduce after some simple computations

$$c_1(x) = c_1^0 + \frac{\varepsilon}{(E - V_n)^{1/4}} \int_{x_n}^{x} \frac{r(y)}{(E - V(y))^{1/4}} sin\left(\frac{1}{\varepsilon} \int_{x_n}^{y} \sqrt{E - V(t)} dt \right) dy\,,$$

and

$$c_2(x) = c_2^0 + \frac{\varepsilon}{(E - V_{n+1})^{1/4}} \int_{x_n}^{x} \frac{r(y)}{(E - V(y))^{1/4}} sin\left(\frac{1}{\varepsilon} \int_{x_{n+1}}^{y} \sqrt{E - V(t)} dt \right) dy\,.$$

The boundary conditions of (4.5) enable us to compute c_1^0 and c_2^0, leading finally to the formula

$$e_{1,h}(x) = \mathcal{E}_1(x) + \mathcal{E}_2(x)\,, \tag{4.6}$$

with

$$\mathcal{E}_1(x) = -\frac{\varepsilon}{(E - V(x))^{1/4}} \int_{x_n}^{x} \frac{r(y)}{(E - V(y))^{1/4}} sin\left(\frac{1}{\varepsilon} \int_{y}^{x} \sqrt{E - V(t)} dt \right) dy\,,$$

$$\mathcal{E}_2(x) = \frac{\varepsilon}{(E - V(x))^{1/4}} \frac{sin(\sigma_n(x))}{sin(\gamma_n)} \int_{x_n}^{x_{n+1}} \frac{r(y)}{(E - V(y))^{1/4}} sin\left(\frac{1}{\varepsilon} \int_{y}^{x_{n+1}} \sqrt{E - V(t)} dt \right) dy\,.$$

Differentiating the interpolation error function yields

$$e'_{1,h}(x) = \mathcal{D}_1(x) + \mathcal{D}_2(x) + \mathcal{D}_3(x) + \mathcal{D}_4(x)\,, \tag{4.7}$$

with

$$\mathcal{D}_1(x) = -(E-V(x))^{1/4} \int_{x_n}^{x} \frac{r(y)}{(E-V(y))^{1/4}} cos\left(\frac{1}{\varepsilon}\int_y^x \sqrt{E-V(t)}dt\right) dy\,,$$

$$\mathcal{D}_2(x) = -\frac{1}{4}\frac{\varepsilon V'(x)}{(E-V(x))^{5/4}} \int_{x_n}^{x} \frac{r(y)}{(E-V(y))^{1/4}} sin\left(\frac{1}{\varepsilon}\int_y^x \sqrt{E-V(t)}dt\right) dy\,,$$

$$\mathcal{D}_3(x) = \frac{1}{4}\frac{\varepsilon V'(x)}{(E-V(x))^{5/4}} \frac{sin(\sigma_n(x))}{sin(\gamma_n)} \int_{x_n}^{x_{n+1}} \frac{r(y)}{(E-V(y))^{1/4}} sin\left(\frac{1}{\varepsilon}\int_y^{x_{n+1}} \sqrt{E-V(t)}dt\right) dy\,,$$

$$\mathcal{D}_4(x) = (E-V(x))^{1/4} \frac{cos(\sigma_n(x))}{sin(\gamma_n)} \int_{x_n}^{x_{n+1}} \frac{r(y)}{(E-V(y))^{1/4}} sin\left(\frac{1}{\varepsilon}\int_y^{x_{n+1}} \sqrt{E-V(t)}dt\right) dy\,.$$

In order to estimate the interpolation error in the $\mathcal{V}$-norm, we shall investigate each of these terms, for the two different cases of a meshsize smaller or larger than the de Broglie wave-length.

Case I: $h_n \le \frac{1}{2}\lambda(x)$ in I_n.
Defining the phase by

$$\sigma(y;x) := \frac{1}{\varepsilon}\int_y^x \sqrt{E-V(t)}dt\,,$$

we shall take advantage in this case of the fact, that the phase is close to zero and thus

$$sin(\sigma(y;x)) = \sigma(y;x)\mathcal{O}(1).$$

As besides $r(y) = \mathcal{O}(1)\psi(y)$, we get easily by using Hypothesis A and the fact that $V \in W^{2,\infty}(a,b)$

$$|\mathcal{E}_1(x)| \le c h_n \sqrt{h_n} ||\psi||_{L^2(I_n)} \quad ; \quad |\mathcal{E}_2(x)| \le c h_n \sqrt{h_n} ||\psi||_{L^2(I_n)}\,.$$

Case II: $h_n > c_0\lambda(x)$ in I_n, with $0 < c_0 \le 1/2$.
The characteristic of this case is, that we are far from $\gamma_n = k\pi$, $\forall k \in \mathbb{N}$, such that

$$c_\gamma \le |sin(\gamma_n)| \le 1\,,$$

leading immediately to

$$|\mathcal{E}_1(x)| \le c\sqrt{h_n}\frac{\varepsilon}{\sqrt{E-V(x)}}||\psi||_{L^2(I_n)} \le c h_n^{3/2}||\psi||_{L^2(I_n)}\,,$$

and similarly

$$|\mathcal{E}_2(x)| \le \frac{c}{c_\gamma}\sqrt{h_n}\frac{\varepsilon}{\sqrt{E-V(x)}}||\psi||_{L^2(I_n)} \le c h_n^{3/2}||\psi||_{L^2(I_n)}\,.$$

Altogether, we have

$$||e_{1,h}||_{L^2(a,b)} \le ch^2||\psi||_{L^2(a,b)}\,, \quad \text{as well as} \quad ||e_{1,h}||_{L^\infty(a,b)} \le ch^2||\psi||_{L^\infty(a,b)}\,,$$

with a constant $c > 0$ independent on ε, E and thus on the wave-length λ.

Next, we estimate the derivative terms:

Case I: $h_n \leq \frac{1}{2}\lambda(x)$ in I_n.
Similar arguments as for the terms $\mathcal{E}_1$, $\mathcal{E}_2$, yield

$$|\mathcal{D}_1(x)| \leq c\sqrt{h_n}||\psi||_{L^2(I_n)} \quad ; \quad |\mathcal{D}_2(x)| \leq ch_n\sqrt{h_n}||\psi||_{L^2(I_n)} \,,$$
$$|\mathcal{D}_3(x)| \leq ch_n\sqrt{h_n}||\psi||_{L^2(I_n)} \quad ; \quad |\mathcal{D}_4(x)| \leq c\sqrt{h_n}||\psi||_{L^2(I_n)} \,,$$

implying for a stepsize smaller than the wavelength

$$||e'_{1,h}||_{L^2(I_n)} \leq ch_n||\psi||_{L^2(I_n)} \,, \quad \text{as well as} \quad ||e'_{1,h}||_{L^\infty(I_n)} \leq ch_n||\psi||_{L^\infty(I_n)} \,.$$

Case II: $h_n > c_0\lambda(x)$ in I_n.
Analogous reasoning as for the terms $\mathcal{E}_1$, $\mathcal{E}_2$, leads to

$$|\mathcal{D}_1(x)| \leq c\sqrt{h_n}||\psi||_{L^2(I_n)} \quad ; \quad |\mathcal{D}_2(x)| \leq c\sqrt{h_n}\frac{\varepsilon}{\sqrt{E-V(x)}}||\psi||_{L^2(I_n)} \leq ch_n^{3/2}||\psi||_{L^2(I_n)} \,,$$
$$|\mathcal{D}_3(x)| \leq \frac{c}{c_\gamma}h_n^{3/2}||\psi||_{L^2(I_n)} \quad ; \quad |\mathcal{D}_4(x)| \leq \frac{c}{c_\gamma}\sqrt{h_n}||\psi||_{L^2(I_n)} \,.$$

Combining these estimates, we deduce in the case of a stepsize larger than the wavelength

$$||e'_{1,h}||_{L^2(I_n)} \leq ch_n||\psi||_{L^2(I_n)} \,, \quad \text{as well as} \quad ||e'_{1,h}||_{L^\infty(I_n)} \leq ch_n||\psi||_{L^\infty(I_n)} \,.$$

Altogether the two cases lead to

$$\frac{\varepsilon}{\sqrt{E+||V||_\infty}}||e'_{1,h}||_{L^2(a,b)} \leq ch\frac{\varepsilon}{\sqrt{E+||V||_\infty}}||\psi||_{L^2(a,b)} \,.$$

∎

The exact solution ψ of the continuous problem (2.1) satisfies the numerical scheme (3.16) with a certain error, the consistency error. Introducing the exact values $\psi(x_n)$ in the discrete scheme, yields the following equation

$$b(\Pi_h\psi, \zeta_n) = L(\zeta_n) + \omega_n \,, \quad \forall n = 1, \dots, N \,,$$

with ω_n the corresponding error terms. Due to the fact that $b(\psi, \zeta_n) = L(\zeta_n)$, we can write

$$\omega_n = b(\Pi_h\psi - \psi, \zeta_n) \,, \quad \forall n = 1, \dots, N \,,$$

and the estimate of this error term is given by the next lemma.

Lemma 4.3 (Consistency result)
Let $V \in W^{2,\infty}(a,b)$ and let Hypothesis A and B be satisfied. The terms $b(\Pi_h\psi - \psi, \zeta_n)$ can be rewritten $\forall n$ under the following form

$$b(\Pi_h\psi - \psi, \zeta_n) = -\frac{\varepsilon^2}{E+||V||_\infty}\int_{x_{n-1}}^{x_{n+1}}\left(\frac{1}{4}\frac{V''(x)}{E-V(x)} + \frac{5}{16}\frac{(V'(x))^2}{(E-V(x))^2}\right)(\Pi_h\psi - \psi)\zeta_n dx \,, \tag{4.8}$$

leading to the estimate

$$|b(\Pi_h \psi - \psi, \zeta_n)| \leq c \frac{\varepsilon^2}{E + ||V||_\infty} ||\Pi_h \psi - \psi||_{L^1(x_{n-1},x_{n+1})} \leq c h^3 \frac{\varepsilon^2}{E + ||V||_\infty} \,,$$

with $c > 0$ *a constant independent on* ε, E *and* $h < h_*$.

Proof: Expression (4.8) is deduced immediately from

$$b(\Pi_h\psi - \psi, \zeta_n) = \frac{\varepsilon^2}{E + ||V||_\infty} \int_a^b (\Pi_h \psi - \psi)' \zeta_n' dx + \frac{1}{E + ||V||_\infty} \int_a^b (V - E)(\Pi_h \psi - \psi) \zeta_n dx \,,$$

by observing that $\zeta_n \in \mathcal{V}_h$ is solution of the equation $\mathcal{A}_{\varepsilon,E} \zeta_n = 0$ in $I_{n-1} \cup I_n$, with the operator $\mathcal{A}_{\varepsilon,E}$ given by (4.4). Using Theorem 4.2 and Lemma 3.2, we get the desired result.

■

4.2 Stability

We shall start with a stability result generalizing the statement given in Theorem 3.5. This result will permit to establish the estimate for the second error term $||\Pi_h^{\varepsilon,E} \psi - \psi_h||_{\mathcal{V}}$.

Theorem 4.4 (Stability result)
Let $V \in W^{2,\infty}(a,b)$ *and let Hypothesis A and B be satisfied. Let moreover* $\phi_h \in \mathcal{V}_h$ *be the solution of the equation*

$$b(\phi_h, \theta_h) = F(\theta_h) \,, \quad \forall \theta_h \in \mathcal{V}_h \,, \tag{4.9}$$

with the antilinear form

$$F(\theta_h) := \frac{\varepsilon^2}{E + ||V||_\infty} \int_a^b f(x) \overline{\theta_h(x)} dx \,, \quad f \in L^\infty(a,b) \,.$$

Then ϕ_h *satisfies the following estimate*

$$||\phi_h||_{\mathcal{V}} \leq c \frac{\varepsilon}{\sqrt{E + ||V||_\infty}} ||f||_{L^\infty(a,b)} \,,$$

with a constant $c > 0$ *independent on* ε, E *and* $h < h_*$.

Proof: Let us decompose $\phi_h \in \mathcal{V}_h$ in terms of the WKB basis functions

$$\phi_h(x) = \sum_{n=1}^N z_n \zeta_n(x).$$

The coefficients z_n are thus solution of the linear system

$$\begin{pmatrix} b(\zeta_1,\zeta_1) & b(\zeta_2,\zeta_1) & \cdots & b(\zeta_N,\zeta_1) \\ b(\zeta_1,\zeta_2) & b(\zeta_2,\zeta_2) & \cdots & b(\zeta_N,\zeta_2) \\ \vdots & \vdots & & \vdots \\ b(\zeta_1,\zeta_N) & b(\zeta_2,\zeta_N) & \cdots & b(\zeta_N,\zeta_N) \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_N \end{pmatrix} = \begin{pmatrix} F(\zeta_1) \\ F(\zeta_2) \\ \vdots \\ F(\zeta_N) \end{pmatrix}, \qquad (4.10)$$

which differs from the linear system (3.16) in the right hand side. Similar as in the proof of Theorem 3.5, we shall start by estimating the coefficients z_n, proceeding in two steps.

1. STEP Estimates on z_1 and z_N.
Choosing in (4.9) as test function $\theta_h := \phi_h$, and taking the imaginary part, yields

$$k_a|z_1|^2 + k_b|z_N|^2 = -\mathcal{I}m \int_a^b f(x)\overline{\phi_h(x)}dx \le ||f||_{L^2(a,b)}||\phi_h||_{L^2(a,b)}. \qquad (4.11)$$

This implies

$$|z_i|^2 \le c\frac{\varepsilon}{\sqrt{E+||V||_\infty}}||f||_{L^\infty(a,b)}||\phi_h||_{L^2(a,b)} \quad \text{for} \quad i=1 \text{ and } i=N\,.$$

2. STEP Estimates on the remaining z_n.
Starting from the last line of the linear system (4.10), we are now able to prove step by step the remaining estimates. We have

$$\begin{aligned} z_{N-1} &= \frac{F(\zeta_N)}{b(\zeta_{N-1},\zeta_N)} - \frac{b(\zeta_N,\zeta_N)}{b(\zeta_{N-1},\zeta_N)}z_N \\ &= T_{N-1} + (\eta_{N-1} + \kappa_{N-1}\sin\gamma_{N-1})(1+\mathcal{O}(h))z_N\,, \end{aligned}$$

with η_{N-1} and κ_{N-1} given by (3.22) and

$$T_{N-1} := \tau_{N-1}\sin\gamma_{N-1}(1+\mathcal{O}(h))\,,$$

where

$$\tau_{N-1} := -\frac{\varepsilon}{\sqrt{E-V_{N-1}}}\int_{x_{N-1}}^{x_N} f(x)\zeta_N dx\,. \qquad (4.12)$$

Let us define $T_N := 0$. By a simple induction we deduce the expression for the coefficient z_{N-i} in terms of z_N, for $i = 2, \dots, N-2$

$$\begin{aligned} z_{N-i} &= \frac{F(\zeta_{N-i+1})}{b(\zeta_{N-i},\zeta_{N-i+1})} - \frac{b(\zeta_{N-i+1},\zeta_{N-i+1})}{b(\zeta_{N-i},\zeta_{N-i+1})}z_{N-i+1} - \frac{b(\zeta_{N-i+2},\zeta_{N-i+1})}{b(\zeta_{N-i},\zeta_{N-i+1})}z_{N-i+2} \\ &= T_{N-i} + (\eta_{N-i} + \kappa_{N-1}\sin(\gamma_{N-1}+\ldots+\gamma_{N-i}) + \ldots + \kappa_{N-i}\sin(\gamma_{N-i}))(1+\mathcal{O}(h))^i z_N \end{aligned}$$

with

$$\begin{aligned} T_{N-i} &:= \tau_{N-1}\sin(\gamma_{N-1}+\ldots+\gamma_{N-i})(1+\mathcal{O}(h))^i + \ldots + \tau_{N-i}\sin(\gamma_{N-i})(1+\mathcal{O}(h)) \\ &= \sum_{l=1}^{i} \tau_{N-l}\sin(\gamma_{N-l}+\ldots+\gamma_{N-i})(1+\mathcal{O}(h))^{i-l+1}\,, \end{aligned} \qquad (4.13)$$

and where the coefficients η_{N-i} and κ_{N-j} are given by (3.23), (3.24). The terms τ_{N-j} have the form

$$\begin{aligned}\tau_{N-j} \;&:=\; -\frac{\varepsilon}{\sqrt{E-V_{N-j}}}\int_{x_{N-j}}^{x_{N-j+2}} f(x)\zeta_{N-j+1}dx\\ &\quad -\frac{\varepsilon}{\sqrt{E-V_{N-j+1}}}\int_{x_{N-j}}^{x_{N-j+2}} W(x)|\zeta_{N-j+1}|^2dx\,T_{N-j+1}\,,\quad j=1,\ldots,N-2\,.\end{aligned}$$

In order to estimate the coefficients z_n, we remark that

$$|T_{N-i}| \le \sum_{l=1}^{i}|\tau_{N-l}|(1+ch)^{i-l+1}\,,\quad i=1,\ldots,N-2\,,$$

and

$$|\tau_{N-l}| \le ch\frac{\varepsilon}{\sqrt{E+||V||_\infty}}||f||_{L^\infty(a,b)} + ch\frac{\varepsilon}{\sqrt{E+||V||_\infty}}|T_{N-l+1}|\,,$$

with constants $c>0$ independent on ε, E and h. Induction arguments yield finally for $l=1,\ldots,N-2$

$$\begin{aligned}|\tau_{N-l}| \;&\le\; ch\frac{\varepsilon}{\sqrt{E+||V||_\infty}}||f||_{L^\infty(a,b)}\left[1+ch\sum_{j=1}^{l-1}(1+ch)^{2j-1}\right]\\ |T_{N-l}| \;&\le\; ch\frac{\varepsilon}{\sqrt{E+||V||_\infty}}||f||_{L^\infty(a,b)}\sum_{j=1}^{l}(1+ch)^{2j-1}\,,\end{aligned}$$

implying with (3.25) for $i=1,\ldots,N-2$

$$\begin{aligned}|z_{N-i}| \;&\le\; |T_{N-i}| + \left(1+\sum_{l=1}^{i}|\kappa_{N-l}|\right)(1+ch)^i|z_N|\\ &\le\; ch\frac{\varepsilon}{\sqrt{E+||V||_\infty}}||f||_{L^\infty(a,b)}\sum_{j=1}^{i}(1+ch)^{2j-1} + (1+\kappa)(1+ch)^{2i-1}|z_N|\\ &\le\; c\frac{\varepsilon}{\sqrt{E+||V||_\infty}}||f||_{L^\infty(a,b)}\frac{(1+ch)^{2i+1}-(1+ch)}{2+ch} + (1+\kappa)(1+ch)^{2i-1}|z_N|\,.\end{aligned}$$

Due to the fact that $(1+ch)^N \to e^c$ for $N\to\infty$, we get

$$|z_n| \le c\frac{\varepsilon}{\sqrt{E+||V||_\infty}}||f||_{L^\infty(a,b)} + c\left(\frac{\varepsilon}{\sqrt{E+||V||_\infty}}||f||_{L^\infty(a,b)}||\phi_h||_{L^2(a,b)}\right)^{1/2}\qquad \forall n\,,$$

with a constant $c>0$ independent on the parameters ε and E and on n. This leads to

$$\begin{aligned}\int_a^b|\phi_h(x)|^2dx &= \sum_{n=1}^{N}\left(z_n\overline{z_{n-1}}\int_{x_{n-1}}^{x_n}\zeta_n\zeta_{n-1}dx + |z_n|^2\int_{x_{n-1}}^{x_{n+1}}|\zeta_n|^2dx + z_n\overline{z_{n+1}}\int_{x_n}^{x_{n+1}}\zeta_n\zeta_{n+1}dx\right)\\ &\le\; c\frac{\varepsilon^2}{E+||V||_\infty}||f||^2_{L^\infty(a,b)} + c\frac{\varepsilon}{\sqrt{E+||V||_\infty}}||f||_{L^\infty(a,b)}||\phi_h||_{L^2(a,b)}\,,\end{aligned}$$

implying with the Young inequality

$$||\phi_h||^2_{L^2(a,b)} \leq c \frac{\varepsilon^2}{E + ||V||_\infty} ||f||^2_{L^\infty(a,b)} \,,$$

with a constant $c > 0$ independent on the parameters ε and E and on the meshsize $h < h_*$. The rest of the proof is straightforward, by observing that

$$\frac{\varepsilon^2}{E + ||V||_\infty} \int_a^b |\phi_h'(x)|^2 dx \leq \int_a^b |\phi_h(x)|^2 dx + \frac{\varepsilon^2}{E + ||V||_\infty} ||f||_{L^2(a,b)} ||\phi_h||_{L^2(a,b)} \,.$$

This inequality is deduced by taking the real part of the equation $b(\phi_h, \phi_h) = F(\phi_h)$.

∎

We proceed now to the study of the second error term $||\Pi_h^{\varepsilon,E}\psi - \psi_h||_{\mathcal{V}}$. Let us denote $e_{2,h}(x) := \Pi_h^{\varepsilon,E}\psi(x) - \psi_h(x)$.

Theorem 4.5 (Error estimate)
Let $V \in W^{2,\infty}(a,b)$. Under Hypothesis A and B, the error between the interpolant of the exact solution and the discrete solution is estimated as follows

$$||\Pi_h^{\varepsilon,E}\psi - \psi_h||_{\mathcal{V}} \leq c \frac{\varepsilon}{\sqrt{E + ||V||_\infty}} h^2,$$

with $h := max_n h_n$ satisfying $h < h_*$, where h_* is independent on ε, E, and with $c > 0$ a constant independent on ε, E and h.

Proof: We start by observing that

$$b(\psi - \psi_h, \theta_h) = 0 \,, \quad \forall \theta_h \in \mathcal{V}_h \,,$$

implying

$$b(\Pi_h\psi - \psi_h, \theta_h) = b(\Pi_h\psi - \psi, \theta_h) = -b(e_{1,h}, \theta_h) \,, \quad \forall \theta_h \in \mathcal{V}_h. \tag{4.14}$$

At this stage, we remark that the term on the right hand side can be rewritten with (4.8) under the following form

$$b(\Pi_h\psi - \psi, \theta_n) = -\frac{\varepsilon^2}{E + ||V||_\infty} \int_a^b \left(\frac{1}{4} \frac{V''(x)}{E - V(x)} + \frac{5}{16} \frac{(V'(x))^2}{(E - V(x))^2} \right) (\Pi_h\psi - \psi) \overline{\theta_n} dx \,,$$

such that using Theorem 4.4 with $f(x) := -W(x)(\Pi_h\psi(x) - \psi(x)) \in L^\infty(a,b)$, W being defined in (3.13), we deduce

$$||\Pi_h^{\varepsilon,E}\psi - \psi_h||_{\mathcal{V}} \leq c \frac{\varepsilon}{\sqrt{E + ||V||_\infty}} ||\Pi_h^{\varepsilon,E}\psi - \psi||_{L^\infty(a,b)} \,.$$

Using now the estimate of Theorem 4.2, we get the desired result.

∎

5 Conclusion

This paper was devoted to the numerical analysis of a finite element scheme, based on the WKB approximation and applied to the 1D stationary Schrödinger equation. The consistency and stability results have proven the convergence of the method in the oscillating case without turning points. The convergence error is shown to be proportional to the meshsize h. The constants involved in the error estimates are independent on the wave-length, which emphasizes the important feature of this method, namely the fact, that a unique multi-wavelength grid is sufficient to get accurate results. In a forthcoming paper, the numerical analysis of the 1D case including turning points shall be treated, as well as the the extention to the 2D case.

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