Convergence analysis of an operator-compressed multiscale finite element method for Schrödinger equations with multiscale potentials

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Abstract

In this paper, we analyze the convergence of the operator-compressed multiscale finite element method (OC MsFEM) for Schrödinger equations with multiscale potentials in the semiclassical regime. The multiscale basis functions are constructed by solving a constrained energy minimization. Under a mild assumption on the mesh size H, we prove the exponential decay of the multiscale basis functions so that localized multiscale basis functions can be constructed. The localized basis functions would achieve the same accuracy as the global ones if the oversampling size $m = O(\log(1/H))$. Based on the properties of Clément-type interpolation, we prove the first-order convergence in the energy norm and second-order convergence in the L^2 norm for the Galerkin approximation in the multiscale finite element space. Furthermore, super convergence rates of second order in the energy norm and third order in the L^2 norm can be obtained if the solution possesses sufficiently high regularity. Finally, we present numerical results to demonstrate the accuracy of the OC MsFEM.

Key words. Schrödinger equation; multiscale potential; multiscale finite element basis; operator compression; convergence analysis.

AMS subject classifications. 65M12, 65M60, 65K10, 35Q41, 74Q10

1. Introduction

In solid state physics, an important model to describe the motion of an electron in the medium with microstructures is the Schrödinger equation with a multiscale potential in the semiclassical regime

$$\begin{cases} i\varepsilon\partial_t u^{\varepsilon,\delta} = -\dfrac{1}{2}\varepsilon^2\Delta u^{\varepsilon,\delta} + V^\delta(\mathbf{x})u^{\varepsilon,\delta}, \quad \mathbf{x} = (x_1, ..., x_d) \in \mathbb{R}^d, \quad t \in \mathbb{R}, \\ u^{\varepsilon,\delta}|_{t=0} = u_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \end{cases} \tag{1.1}$$

where $0 < \varepsilon \ll 1$ is an effective Planck constant describing the microscopic/macroscopic scale ratio, d is the spatial dimension, $V^\delta(\mathbf{x}) \in \mathbb{R}$ is a multiscale potential depending on another small parameter $0 < \delta \ll 1$, and $u_0(\mathbf{x})$ is the initial data.

A widely studied model is the electron motion in a perfect crystal with an external field, where $V^\delta(\mathbf{x}) = V^\varepsilon(\mathbf{x}) = V_1(\frac{\mathbf{x}}{\varepsilon}) + V_2(\mathbf{x})$ with $V_1(\frac{\mathbf{x}}{\varepsilon})$ as an oscillatory periodic potential and $V_2(\mathbf{x})$

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as an external field. This model can be efficiently solved by a number of numerical schemes that make use of the periodic structure of the potential, e.g. the Bloch decomposition-based time-splitting pseudospectral method [19, 20, 42], the Gaussian beam method [24, 25, 38, 43], and the frozen Gaussian approximation method [8]. With the recent development in nanotechnology, increasing interest has been shown in quantum heterostructures with tailored functionalities, such as heterojunctions, including the ferromagnet/metal/ferromagnet structure for giant megnetoresistance [44], the silicon-based heterojunction for solar cells [27], and quantum metamaterials [39]. For the electron motion in these heterostructures, however, the potential $V^\delta(\mathbf{x})$ cannot be formulated in the above-mentioned form since a basic feature of these devices is the combination of dissimilar crystalline structures, which leads to a heterogeneous interaction of the electron with ionic cores in different lattice structures. Consequently, available methods based on asymptotic analysis [31, 32] cannot be applied to these heterogeneous models since these methods require an additive form of different scales in the potential term in order to construct the prescribed approximate solutions. Moreover, for a general multiscale potential $V^\delta(\mathbf{x})$, traditional methods like the finite element method [9] and finite difference method [29, 30] are prohibitively costly due to the strong mesh size restrictions induced by the multiscale structure in the potential, while the time-splitting spectral method [1] would suffer from reduced convergence order and great approximation errors if the potential possesses discontinuities.

In order to efficiently compute (1.1) with the multiscale potential $V^\delta(\mathbf{x})$ in a general form, an operator-compressed multiscale finite element method (OC MsFEM) for the Schrödinger equation was proposed in [4]. The OC MsFEM for the Schrödinger equation is motivated by several works relevant to the compression of the elliptic operator with heterogeneous and highly varying coefficients, e.g. the multigrid method for multiscale problems from the perspective of a decision theory discussed in [33, 34], the sparse operator compression of high-order elliptic operators with rough coefficients studied in [18] and the modified variational multiscale method using correctors introduced in [28]. And we remark here that many efficient methods have also been developed for the multiscale PDEs in the past few decades. See for example [5, 10, 11, 15, 17, 22, 23, 26, 35] and the references therein.

In the OC MsFEM for the Schrödinger equation, the multiscale basis functions are constructed via a constrained energy minimization associated with the hamiltonian $\mathcal{H} = -\frac{1}{2}\varepsilon^2\Delta + V^\delta(\mathbf{x})$. The fully discrete scheme can be given with a finite difference scheme in temporal discretization, e.g. the backward Euler or Crank-Nicolson scheme. Through the energy minimization, the local microstructures induced by the hamiltonian $\mathcal{H}$ are incorporated in the basis functions so that the multiscale features of the solution are well captured by the basis functions. Moreover, the energy minimization can be solved numerically without any assumptions on the multiscale potential V^δ and thus the OC MsFEM for the Schrödinger equation can be applied for a multiscale potential V^δ in a general form. In [4], the OC MsFEM is shown to be accurate for various types of multiscale potentials. So far, however, there have been no rigorous results on the approximation error of the OC MsFEM for the Schrödinger equation.

In this paper, we focus on the convergence analysis of the OC MsFEM for Schrödinger equations with multiscale potentials in the semiclassical regime. The property of exponential decay is proved for the multiscale basis functions constructed through the constrained energy minimization, provided that the mesh size $H = O(\varepsilon)$. Thus the localized multiscale basis functions can be constructed via a modified constrained energy minimization. The localized basis functions are shown to admit the same accuracy as the global ones if the oversampling size $m = O(\log(1/H))$. By using the properties of Clément-type interpolation [2, 7, 40], convergence rates of first order in the energy norm and second order in L^2 norm are proved for the Galerkin approximation in the multiscale finite element space. Furthermore, super convergence rates of second order in the energy norm and third order in L^2 norm can be achieved if the solution possesses sufficiently high regularity. Combining the analysis on the regularity of the solution, we also derive the dependence of the error bounds on the small parameters ε and δ. We find that using the same mesh size the OC MsFEM gives more accurate results than the FEM for the Schrödinger equation with multiscale potentials due to its super convergence behavior and weaker dependence on the small parameters ε, δ. Finally, we present numerical results to confirm our theoretical findings.

The rest of the paper is organized as follows. In Section 2, the problem setting and some preliminaries on the regularity of the solution and the Clément-type interpolation will be introduced. The exponential decay of the global basis functions will be proved and the approximation property of the projection in both global and localized multiscale space will be discussed in Section 3. The convergence rates of the OC MsFEM for the Schrödinger equation will be given in Section 4. And a few numerical examples will be shown in Section 5 to support our analysis. Finally, some conclusions will be drawn in Section 6.

2. Problem setting and some preliminaries

In this section, the problem setting of the Schrödinger equation with a multiscale potential is formulated. Then the regularity of the solution is discussed. And some results on the Clément-type interpolation are introduced.

All functions are complex-valued and the conjugate of a function v is denoted by $\bar{v}$. Standard notations on Sobolev space are used. The spatial derivative is denoted by $D_{\mathbf{x}}^{\boldsymbol{\sigma}}$, where $D_{\mathbf{x}}^{\boldsymbol{\sigma}} w = \partial_{x_1}^{\sigma_1} \cdots \partial_{x_d}^{\sigma_d} w$ with the multi-index $\boldsymbol{\sigma} = (\sigma_1, \dots, \sigma_d) \in \mathbb{N}^d$ and $|\boldsymbol{\sigma}| = \sigma_1 + \cdots + \sigma_d$. The spatial L^2 inner product is denoted by $(\cdot,\cdot)$ with $(v, w) = \int_\Omega v\bar{w}$, the spatial L^2 norm is denoted by $||\cdot||$ with $||w||^2 = (w, w)$, $||\cdot||_\infty$ is the spatial L^∞ norm with $||w||_\infty = \operatorname{ess\,sup}_{\mathbf{x}\in\Omega} |w(\mathbf{x})|$ and the spatial H^k norm is denoted by $||\cdot||_{H^k}$ with $||w||_{H^k}^2 = ||w||^2 + \sum_{0<|\boldsymbol{\sigma}|\le k} ||D_{\mathbf{x}}^{\boldsymbol{\sigma}} w||^2$. And we define $H_P^1(\Omega) = \{w \in H^1(\Omega) | w \text{ is periodic on } \partial\Omega\}$, where Ω is a bounded domain. To simplify notations, we denote by C a generic positive constant which may be different at each occurrence but is independent of the small parameters ε, δ, the oversampling size m, the spatial mesh size H and the time step size Δt.

2.1. Model setting

For numerical purposes, (1.1) is restricted on a bounded domain $\Omega = [0, 2\pi]^d$ with prescribed periodic boundary conditions. The following problem is considered:

$$\begin{cases} i\varepsilon\partial_t u^{\varepsilon,\delta} = -\dfrac{1}{2}\varepsilon^2 \Delta u^{\varepsilon,\delta} + V^\delta(\mathbf{x}) u^{\varepsilon,\delta}, \quad \mathbf{x} \in \Omega, 0 < t \le T, \\ u^{\varepsilon,\delta}, D_{\mathbf{x}}^{\boldsymbol{\sigma}} u^{\varepsilon,\delta} \text{ are periodic on } \partial\Omega, \quad |\boldsymbol{\sigma}| = 1, 0 < t \le T, \\ u^{\varepsilon,\delta}|_{t=0} = u_0(\mathbf{x}), \mathbf{x} \in \Omega. \end{cases} \tag{2.1}$$

We assume that $u_0(\mathbf{x})$ is smooth and independent of the small parameters ε, δ. And for the multiscale potential V^δ, we assume that $V_{\min} \le V^\delta(\mathbf{x}) \le V_{\max}$, $\forall \mathbf{x} \in \Omega$, where $0 < V_{\min} \le V_{\max}$ and $|D_{\mathbf{x}}^{\boldsymbol{\sigma}} V^\delta| \le \frac{C}{\delta^{|\boldsymbol{\sigma}|}}$, $\forall \mathbf{x} \in \Omega$. We additionally assume that $D_{\mathbf{x}}^{\boldsymbol{\sigma}} u^{\varepsilon,\delta}$ are periodic on $\partial\Omega$ for $|\boldsymbol{\sigma}| = 2, 3$ and $0 < t \le T$.

Remark 2.1. If $\tilde{u}^{\varepsilon,\delta}$ is the solution of (2.1) with the potential $\tilde{V}^\delta$, where $-V_0 \le \tilde{V}^\delta \le V_0$ for some $V_0 > 0$, we may set $u^{\varepsilon,\delta} = e^{-2iV_0 t/\varepsilon} \tilde{u}^{\varepsilon,\delta}$. Then $u^{\varepsilon,\delta}$ is the solution of (2.1) with the potential $V^\delta = \tilde{V}^\delta + 2V_0$ and $V_0 \le V^\delta \le 3V_0$.

In what follows, for brevity of notations, the superscripts ε, δ will be dropped for $u^{\varepsilon,\delta}$ and V^δ unless necessary. We introduce the bilinear form associated with the Schrödinger operator $\mathcal{H} = -\frac{1}{2}\varepsilon^2\Delta + V$ as

$$a(v, w) = \frac{1}{2}\varepsilon^2(\nabla v, \nabla w) + (Vv, w). \tag{2.2}$$

The following energy norm is introduced:

$$||w||_e = a(w, w)^{\frac{1}{2}} = \left(\frac{\varepsilon^2}{2}||\nabla w||^2 + (Vw, w)\right)^{\frac{1}{2}}. \tag{2.3}$$

Then, the energy norm $||\cdot||_e$ is equivalent to the H^1 norm $||\cdot||_{H^1}$ and it is easy to prove the following lemma.

Lemma 2.1. For any $v, w \in H^1(\Omega)$,

$$|a(v, w)| \le ||v||_e||w||_e. \tag{2.4}$$

If the stationary problem with $\mathcal{H}$ as the differential operator

$$\begin{cases} \mathcal{H}u = f, \quad \mathbf{x} \in \Omega, \\ u, D_{\mathbf{x}}^{\boldsymbol{\sigma}} u \text{ are periodic on } \partial\Omega, |\boldsymbol{\sigma}| = 1, \end{cases} \tag{2.5}$$

is considered, where periodic boundary conditions are prescribed and $f \in L^2(\Omega)$, the associated variational problem would be to find $u \in H_P^1(\Omega)$ such that

$$a(u, v) = (f, v), \quad \forall v \in H_P^1(\Omega). \tag{2.6}$$

By the Lax-Milgram theorem, the variational problem (2.6) admits a unique solution $u \in H_P^1(\Omega)$ with a stability estimate

$$||u||_e \le C_{\mathrm{st}}(\varepsilon, V)||f||. \tag{2.7}$$

2.2. Regularity of the solutions of Schrödinger equations with multiscale potentials

We first study the temporal regularity of the solution u of the Schrödinger equation (2.1).

Lemma 2.2. If $\partial_t^k u(t) \in L^2(\Omega)$ for any $t \in [0, T]$, where $k = 1, 2, 3, 4$, then it holds true for any $0 \le t \le T$ that

$$||\partial_t^k u(t)|| \le \frac{C\varepsilon^{k-2}}{\min\{\varepsilon^{2k-2}, \delta^{2k-2}\}}. \tag{2.8}$$

Proof. For u_t, taking the time derivative of (2.1), multiplying it with $\bar{u}_t$, integrating it w.r.t. $\mathbf{x}$ over Ω and taking the imaginary part, we have $\frac{d}{dt}||u_t||^2 = 0$, which implies $||u_t(t)|| = ||u_t(0)||, \forall t \in [0,T]$. For $||u_t(0)||$, we have $i\varepsilon u_t(0) = -\frac{\varepsilon^2}{2}\Delta u_0 + Vu_0$, which indicates

$$||u_t(0)|| \leq \frac{\varepsilon}{2}||\Delta u_0|| + \frac{1}{\varepsilon}||Vu_0|| \leq \frac{C}{\varepsilon}. \tag{2.9}$$

Applying similar procedures to u_{tt}, u_{ttt} and u_{tttt}, we can obtain the results (2.8). □

Then, we turn to the spatial regularity of u.

Lemma 2.3. If $D^{\boldsymbol{\sigma}}_{\mathbf{x}} u(t) \in L^2(\Omega)$ for any $t \in [0,T]$ and $|\boldsymbol{\sigma}| = k$, where $k = 1, 2$, then it holds true for any $0 \leq t \leq T$ that

$$||D^{\boldsymbol{\sigma}}_{\mathbf{x}} u(t)|| \leq \frac{C}{\varepsilon^k \delta^k}. \tag{2.10}$$

Proof. For $|\boldsymbol{\sigma}| = 1$, it is sufficient to prove (2.10) for u_{x_1}. We have $||u(t)|| = ||u_0||$ for any $t \in [0,T]$, which is the conservation of mass. Taking the spatial partial derivative of (2.1) w.r.t. x_1, multiplying it with $\bar{u}_{x_1}$, integrating it w.r.t. $\mathbf{x}$ over Ω and taking the imaginary part, we have

$$\varepsilon \frac{1}{2}\frac{d}{dt}||u_{x_1}||^2 = \mathrm{Im}(V_{x_1} u, u_{x_1}). \tag{2.11}$$

Then

$$\frac{1}{2}\frac{d}{dt}||u_{x_1}||^2 = ||u_{x_1}||\frac{d}{dt}||u_{x_1}|| \leq \frac{1}{\varepsilon}|(V_{x_1}u, u_{x_1})| \leq \frac{1}{\varepsilon\delta}||u||||u_{x_1}||, \tag{2.12}$$

and hence $\frac{d}{dt}||u_{x_1}|| \leq \frac{1}{\varepsilon\delta}||u||$. Therefore, we have

$$||u_{x_1}(t)|| \leq ||\partial_{x_1} u_0|| + \frac{T}{\varepsilon\delta}||u_0|| \leq \frac{C}{\varepsilon\delta}, \quad \forall t \in [0,T], \tag{2.13}$$

which implies (2.10) for $|\boldsymbol{\sigma}| = 1$. Then, applying the same procedure to any $D^{\boldsymbol{\sigma}}_{\mathbf{x}} u$ with $|\boldsymbol{\sigma}| = 2$, we obtain the result. □

Furthermore, we have

Lemma 2.4. If $\partial^k_t u(t) \in H^1(\Omega)$ for any $t \in [0,T]$, where $k = 1, 2, 3$, then it holds true for any $0 \leq t \leq T$ that

$$||\nabla \partial^k_t u(t)|| \leq \frac{C\varepsilon^{k-2}}{\varepsilon\delta \min\{\varepsilon^{2k-2}, \delta^{2k-2}\}}. \tag{2.14}$$

Proof. By combining the proofs of Lemmas 2.2 and 2.3, we can obtain the result. □

2.3. Clément-type interpolation

Let $\mathcal{T}_H = \{T_e\}_{e=1}^{N_e}$ be some quasi-uniform and shape-regular simplicial finite element mesh [6, 13, 14] of Ω with mesh size H, where N_e is the number of elements. Then for K being the union of some elements in $\mathcal{T}_H$, the neighbourhood of K can be defined as

$$N(K) = \bigcup_{G \in \mathcal{T}_H, G \cap K \neq \emptyset} G. \tag{2.15}$$

And for $m \in \mathbb{N}$, $N^{m+1}(K) = N(N^m(K))$, where $N^0(K) = K$, and m is referred to as the oversampling size. If we define

$$\eta(\mathbf{x}) = \frac{\mathrm{dist}(\mathbf{x}, N^m(K))}{\mathrm{dist}(\mathbf{x}, N^m(K)) + \mathrm{dist}(\mathbf{x}, \Omega \backslash N^{m+1}(K))} \tag{2.16}$$

for some $m \in \mathbb{N}$, the shape regularity of $\mathcal{T}_H$ implies that $H||\nabla \eta||_\infty \leq \gamma$, where γ is independent of ε, δ, m and H. The shape regularity and quasi-uniformness also imply that there exists a constant C_{ol} independent of ε, δ, m and H [36, 37] such that

$$\max_{T \in \mathcal{T}_H} \mathrm{card}\{G \in \mathcal{T}_H | G \subset N(T)\} \leq C_{\mathrm{ol}}. \tag{2.17}$$

The first-order conforming finite element space of $\mathcal{T}_H$ is given by

$$\Phi_H = \{\phi \in H^1_P(\Omega) | \forall T \in \mathcal{T}_H, \phi|_T \text{ is a polynomial of total degree } \leq 1\}. \tag{2.18}$$

Let $\mathcal{N}_H$ be the set of vertices of $\mathcal{T}_H$ with repeated vertices due to the periodic boundary conditions removed and $N_H = |\mathcal{N}_H|$. Then $\Phi_H = \mathrm{span}\{\phi_j, j = 1, \ldots, N_H\}$, where $\phi_j \in \Phi_H, j = 1, \ldots, N_H$ is the nodal basis satisfying $\phi_j(\mathbf{x}_k) = \delta_{jk}$, $\forall \mathbf{x}_k \in \mathcal{N}_H$. The Clément-type interpolation operator I_H [2, 7, 40] is defined by

$$I_H v = \sum_{j=1}^{N_H} \alpha_j(v) \phi_j, \quad \forall v \in H^1_P(\Omega), \tag{2.19}$$

where $\alpha_j(v) = \frac{(v, \phi_j)}{(1, \phi_j)}$. Then, the local approximation and stability properties of the interpolation operator I_H [3] guarantee that there exists a constant C_{I_H} only dependent on the shape regularity such that

$$H^{-1}||v - I_H v||_T + ||\nabla(v - I_H v)||_T \leq C_{I_H} ||\nabla v||_{N(T)}, \quad \forall T \in \mathcal{T}_H, \tag{2.20}$$

where $(v, w)_K = \int_K v\bar{w}$ and $||v||_K^2 = (v, v)_K$ denote the spatial L^2 inner product and spatial L^2 norm restricted on $K \subset \Omega$ respectively. Set $W = \ker(I_H)$. Then $H^1_P(\Omega) = \Phi_H \oplus W$ and $(v, w) = 0$, $\forall v \in \Phi_H, w \in W$. Finally, we have the following lemma.

Lemma 2.5. For $v \in W, f \in L^2(\Omega)$, there holds

$$(f, v) \leq CH||f||||\nabla v||. \tag{2.21}$$

Moreover, if $f \in H^1(\Omega)$, then

$$(f, v) \leq CH^2||\nabla f||||\nabla v||. \tag{2.22}$$

Proof. Since $v \in W$, then $I_H v = 0$. By (2.17) and (2.20),

$$(f, v) = (f, v - I_H v) \leq ||f||||v - I_H v|| \leq CH||f||||\nabla v||. \tag{2.23}$$

Note that $(I_H f, v) = 0$. Hence if we further have $f \in H^1(\Omega)$, then

$$(f, v) = (f - I_H f, v - I_H v) \leq CH^2||\nabla f||||\nabla v||. \tag{2.24}$$

□

Moreover, there exists a local right inverse of I_H [16], denoted by $I_H^{-1,\mathrm{loc}} : \Phi_H \to H_P^1(\Omega)$, satisfying

$$I_H(I_H^{-1,\mathrm{loc}} v_H) = v_H, \tag{2.25}$$

$$||\nabla I_H^{-1,\mathrm{loc}} v_H|| \le C'_{I_H} ||\nabla v_H||, \tag{2.26}$$

$$\mathrm{supp}(I_H^{-1,\mathrm{loc}} v_H) = \bigcup \{T \in \mathcal{T}_H | T \cap \overline{\mathrm{supp}(v_H)} \ne \emptyset\}, \tag{2.27}$$

where $v_H \in \Phi_H$ and C'_{I_H} only depends on the shape regularity.

3. OC multiscale finite element basis functions for the Schrödinger operator

In this section, the constructions of global and localized multiscale finite element spaces will be introduced. The stationary problem (2.5) will be considered. And the projection errors of the solution u of (2.5) in both the global and localized multiscale finite element spaces will be deduced. Throughout this paper, a resolution assumption is made.

Assumption 3.1. The mesh size H satisfies $H/\varepsilon \le \left(2C_{I_H}\sqrt{C_{\mathrm{ol}} V_{\max}(1 + C_{I_H} C_{\mathrm{ol}} \gamma)}\right)^{-1}$.

Under Assumption 3.1, we have a property for the kernel W.

Lemma 3.1. Under Assumption 3.1, for any $v \in W$

$$\varepsilon ||\nabla v|| \le ||v||_e \le C\varepsilon ||\nabla v||. \tag{3.1}$$

Proof. For any $v \in W$, it is easy to see that $\varepsilon||\nabla v|| \le ||v||_e$. On the other hand, by Lemma 2.5,

$$||v||_e^2 \le \frac{\varepsilon^2}{2}||\nabla v||^2 + V_{\max}(v, v) \le C\left(1 + \frac{H^2}{\varepsilon^2}\right)\varepsilon^2||\nabla v||^2 \le C\varepsilon||\nabla v||, \tag{3.2}$$

which completes the proof. □

3.1. Global multiscale finite element basis functions

For $j = 1, \ldots, N_H$, the operator-compressed multiscale basis function ψ_j is constructed as the solution of the constrained optimization problem

$$\begin{aligned} \min_{\psi \in H_P^1(\Omega)} \quad & a(\psi, \psi), \\ \text{s.t.} \quad & (\psi, \phi_k) = \delta_{jk}, \quad k = 1, \ldots, N_H. \end{aligned} \tag{3.3}$$

Define $\Psi_H = \mathrm{span}\{\psi_j, j = 1, \ldots, N_H\}$ as the global multiscale finite element space. And we have the following lemma.

Lemma 3.2. $H_P^1(\Omega) = \Psi_H \oplus W$ and for any $v_H \in \Psi_H$ and $w \in W$,

$$a(v_H, w) = 0. \tag{3.4}$$

Proof. For any nontrivial $w \in W$ and $\eta \in \mathbb{R}$, $\psi_j + \eta w$ satisfies the constraint in the optimization problem (3.3), $j = 1, \ldots, N_H$. Then

$$g(\eta) = a(\psi_j + \eta w, \psi_j + \eta w) = \eta^2 a(w, w) + 2\eta \text{Re } a(\psi_j, w) + a(\psi_j, \psi_j). \tag{3.5}$$

Since $g(\eta)$ achieves the minimum at $\eta = 0$, then $g'(\eta)|_{\eta=0} = 0$. And hence Re $a(\psi_j, w) = 0$. Set $\tilde{\eta} = i\eta$ and $\tilde{g}(\eta) = g(\tilde{\eta})$. A similar argument for $\tilde{g}(\eta)$ yields that Im $a(\psi_j, w) = 0$. And hence $a(\psi_j, w) = 0$, $j = 1, \ldots, N_H$, i.e.,

$$a(v_H, w) = 0, \quad \forall v_H \in \Psi_H, w \in W. \tag{3.6}$$

For any $v \in H_P^1(\Omega)$, define $v^* = \sum_{k=1}^{N_H} (v, \phi_k)\psi_k$. Then $v^* \in \Psi_H$ and

$$(v - v^*, \phi_j) = 0, \quad j = 1, \ldots, N_H. \tag{3.7}$$

Then $v - v^* \in W$ and hence $H_P^1(\Omega) = \Psi_H \oplus W$. □

To solve the stationary problem (2.5) in Ψ_H, the Galerkin method seeks $u_H \in \Psi_H$ such that

$$a(u_H, v_H) = (f, v_H), \quad \forall v_H \in \Psi_H. \tag{3.8}$$

Then Lemma 3.2 indicates the following lemma.

Lemma 3.3. Assume that u is the solution of (2.5) and u_H is the solution of the Galerkin approximation (3.8) in Ψ_H. Then $u - u_H \in W$.

Proof. By Lemma 3.2, $u - u_H \in W$ since $a(u - u_H, w_H) = 0, \forall w_H \in \Psi_H$. □

We are now in the position to prove the error estimates for u_H.

Theorem 3.1. Let u be the solution of (2.5) and u_H be the solution of (3.8). If $f \in L^2(\Omega)$, then

$$||u - u_H||_e \leq C\frac{H}{\varepsilon}||f||, \tag{3.9}$$

$$||u - u_H|| \leq C\frac{H^2}{\varepsilon^2}||f||. \tag{3.10}$$

Moreover, if $f \in H^1(\Omega)$, then

$$||u - u_H||_e \leq C\frac{H^2}{\varepsilon}||\nabla f||, \tag{3.11}$$

$$||u - u_H|| \leq C\frac{H^3}{\varepsilon^2}||\nabla f||. \tag{3.12}$$

Proof. We first consider the case where $f \in L^2(\Omega)$. For the error in the energy norm, since $u - u_H \in W$, then by Lemma 2.5,

$$\begin{aligned} ||u - u_H||_e^2 &= a(u - u_H, u - u_H) = a(u, u - u_H) \\ &= (f, u - u_H) \leq CH||f||||\nabla(u - u_H)|| \leq C\frac{H}{\varepsilon}||f||||u - u_H||_e. \end{aligned} \tag{3.13}$$

For the L^2 error, the Aubin-Nitsche technique is applied. Let $w \in H^1_P(\Omega)$ be the solution of

$$a(w, v) = (u - u_H, v), \forall v \in H^1_P(\Omega) \tag{3.14}$$

and $w_H \in \Psi_H$ be the Galerkin approximation of w in Ψ_H satisfying

$$a(w_H, v_H) = (u - u_H, v_H), \forall v_H \in \Psi_H. \tag{3.15}$$

Then

$$\begin{aligned} ||u - u_H||^2 &= a(w, u - u_H) = a(w - w_H, u - u_H) \\ &\leq ||w - w_H||_e ||u - u_H||_e \leq C\frac{H^2}{\varepsilon^2}||f||||u - u_H||, \end{aligned} \tag{3.16}$$

where in the last equality we have used the estimate (3.9). Moreover, if $f \in H^1(\Omega)$, we have by Lemma 2.5 that

$$||u - u_H||_e^2 = (f, u - u_H) \leq CH^2||\nabla f||||\nabla(u - u_H)||. \tag{3.17}$$

By repeating the above procedure, we obtain the results (3.11) and (3.12). □

3.2. Localized multiscale finite element basis functions

One advantage of using these operator-compressed multiscale basis functions is that these basis functions have the property of exponential decay, which motivates us to use the localized basis functions constructed by a modified constrained energy minimization in practical computations. In this subsection, we will prove the exponential decay of the operator-compressed multiscale basis functions. Then, we will introduce the construction of localized basis functions and prove the projection error in the multiscale finite element space spanned by these localized basis functions.

3.2.1. Exponential decay of basis functions

Let $S_j = \text{supp}(\phi_j)$. We have the following theorem indicating the exponential decay of basis functions ψ_j.

Theorem 3.2. Under Assumption 3.1, there exists $0 < \beta < 1$ independent of $\varepsilon, \delta, m, H$ such that for all $j = 1, \dots, N_H$ and $m \in \mathbb{N}$,

$$||\nabla\psi_j||_{\Omega\backslash N^m(S_j)} \leq \beta^m||\nabla\psi_j||. \tag{3.18}$$

Proof. In this proof, we fix the index j and omit j for ψ_j and S_j for brevity of notations. Assume $m \geq 7$. Define the cutoff function

$$\eta = \frac{\text{dist}(\mathbf{x}, N^{m-4}(S))}{\text{dist}(\mathbf{x}, N^{m-4}(S)) + \text{dist}(\mathbf{x}, \Omega\backslash N^{m-3}(S))}. \tag{3.19}$$

Then $\eta = 0$ in $N^{m-4}(S)$, $\eta = 1$ in $\Omega\backslash N^{m-3}(S)$ and $0 \leq \eta \leq 1$ in $N^{m-3}(S)\backslash N^{m-4}(S)$. Moreover, $H||\nabla\eta||_\infty \leq \gamma$ and $\mathcal{R} := \text{supp}(\nabla\eta) = N^{m-3}(S)\backslash N^{m-4}(S)$. Then

$$\begin{aligned} ||\nabla\psi||^2_{\Omega\backslash N^m(S)} &\leq (\nabla\psi, \eta\nabla\psi) = (\nabla\psi, \nabla(\eta\psi)) - (\nabla\psi, \psi\nabla\eta) \\ &\leq |(\nabla\psi, \nabla(\eta\psi - I_H^{-1,\text{loc}}(I_H(\eta\psi))))| + |(\nabla\psi, \nabla I_H^{-1,\text{loc}}(I_H(\eta\psi)))| + |(\nabla\psi, \psi\nabla\eta)| \\ &= M_1 + M_2 + M_3, \end{aligned} \tag{3.20}$$

where $M_1 = |(\nabla\psi, \nabla(\eta\psi - I_H^{-1,\mathrm{loc}}(I_H(\eta\psi))))|$, $M_2 = |(\nabla\psi, \nabla I_H^{-1,\mathrm{loc}}(I_H(\eta\psi)))|$, and $M_3 = |(\nabla\psi, \psi\nabla\eta)|$. For M_1, note that $w = \eta\psi - I_H^{-1,\mathrm{loc}}(I_H(\eta\psi)) \in W$, which implies $a(\psi, w) = 0$ and that $\mathrm{supp}(w) \subset \Omega\backslash N^{m-6}(S)$, $\mathrm{supp}(I_H(\eta\psi)) = N^{m-2}(S)\backslash N^{m-5}(S)$, $\mathrm{supp}(\eta\psi - I_H(\eta\psi)) \subset \Omega\backslash N^{m-5}(S)$, $\mathrm{supp}(I_H(\eta\psi) - I_H^{-1,\mathrm{loc}}(I_H(\eta\psi))) \subset N^{m-1}(S)\backslash N^{m-6}(S)$. Hence

$$\begin{aligned} M_1 &\leq \frac{2V_{\max}}{\varepsilon^2}|(\psi, w)| = \frac{2V_{\max}}{\varepsilon^2}|(\psi - I_H\psi, \eta\psi - I_H(\eta\psi) + I_H(\eta\psi) - I_H^{-1,\mathrm{loc}}(I_H(\eta\psi)))| \\ &\leq \frac{2V_{\max}}{\varepsilon^2}\left(|(\psi - I_H\psi, \eta\psi - I_H(\eta\psi))| + |(\psi - I_H\psi, I_H(\eta\psi) - I_H^{-1,\mathrm{loc}}(I_H(\eta\psi)))|\right) \\ &\leq 2V_{\max}C_{I_H}^2 C_{\mathrm{ol}}\frac{H^2}{\varepsilon^2}||\nabla\psi||_{\Omega\backslash N^{m-6}(S)}||\nabla(\eta\psi)||_{\Omega\backslash N^{m-6}(S)} \\ &+ 2V_{\max}C_{I_H}^3 C'_{I_H} C_{\mathrm{ol}}\frac{H^2}{\varepsilon^2}||\nabla\psi||_{N^m(S)\backslash N^{m-7}(S)}||\nabla(\eta\psi)||_{N^m(S)\backslash N^{m-7}(S)}. \end{aligned} \tag{3.21}$$

Also note that $\mathcal{R} \cap \mathrm{supp}(I_H\psi) = \emptyset$ and hence

$$||\psi\nabla\eta||_{\mathcal{R}} = ||(\psi - I_H\psi)\nabla\eta||_{\mathcal{R}} \leq C_{I_H}C_{\mathrm{ol}}H||\nabla\eta||_\infty||\nabla\psi||_{N(\mathcal{R})} \leq C_{I_H}C_{\mathrm{ol}}\gamma||\nabla\psi||_{N(\mathcal{R})}. \tag{3.22}$$

Thus under Assumption 3.1, we arrive at

$$M_1 \leq \frac{1}{2}||\nabla\psi||^2_{\Omega\backslash N^m(S)} + C||\nabla\psi||^2_{N^m(S)\backslash N^{m-7}(S)}. \tag{3.23}$$

Using a similar argument, we have

$$M_2 \leq C||\nabla\psi||_{N^{m-1}(S)\backslash N^{m-6}(S)}||\nabla(\eta\psi)||_{N^{m-1}(S)\backslash N^{m-6}(S)} \leq C||\nabla\psi||^2_{N^m(S)\backslash N^{m-7}(S)}, \tag{3.24}$$

$$M_3 \leq C||\nabla\psi||^2_{N^m(S)\backslash N^{m-7}(S)}. \tag{3.25}$$

And hence

$$\frac{1}{2}||\nabla\psi||^2_{\Omega\backslash N^m(S)} \leq C_1||\nabla\psi||^2_{N^m(S)\backslash N^{m-7}(S)}, \tag{3.26}$$

where C_1 is independent of ε, δ, m and H. And this leads to

$$||\nabla\psi||^2_{\Omega\backslash N^m(S)} \leq \frac{C_1}{C_1 + \frac{1}{2}}||\nabla\psi||^2_{\Omega\backslash N^{m-7}(S)}, \tag{3.27}$$

which implies

$$||\nabla\psi||^2_{\Omega\backslash N^m(S)} \leq \left(\frac{C_1}{C_1 + \frac{1}{2}}\right)^{\lfloor \frac{m}{7} \rfloor}||\nabla\psi||^2. \tag{3.28}$$

□

3.2.2. Localized basis functions

Motivated by the exponential decay of the multiscale basis functions, we can construct the localized basis function $\psi_j^{\mathrm{loc},m}$ by solving the modified constrained optimization problem

$$\begin{aligned} \min_{\psi \in H^1_P(\Omega)} \quad & a(\psi, \psi), \\ \text{s.t.} \quad & (\psi, \phi_k) = \delta_{jk}, \quad k = 1, \ldots, N_H, \\ & \psi(\mathbf{x}) = 0, \quad \text{for } \mathbf{x} \in \Omega\backslash N^m(S_j) \end{aligned} \tag{3.29}$$

for $j = 1, \ldots, N_H$ and $m \in \mathbb{N}$. Let $W(N^m(S_j)) = \{w \in W | w = 0 \text{ in } \Omega \backslash N^m(S_j)\}$. Following the proof of Lemma 3.2, we have

Lemma 3.4. It holds true that for $j = 1, \ldots, N_H$

$$a(\psi_j^{\text{loc},m}, w) = 0, \quad \forall w \in W(N^m(S_j)). \tag{3.30}$$

Define $\Psi_{H,m} = \text{span}\{\psi_j^{\text{loc},m}, j = 1, \ldots, N_H\}$ as the localized multiscale finite element space. Before we study the projection error in $\Psi_{H,m}$, a lemma on the bound of $||\nabla \psi_j||$ is needed.

Lemma 3.5. Under Assumption 3.1, it holds true that for $j = 1, \ldots, N_H$

$$||\nabla \psi_j|| \leq CH^{-\frac{3}{2}d}. \tag{3.31}$$

Proof. Define the operator P as for any $v \in H_P^1(\Omega)$, $Pv \in W$ and

$$a(Pv, w) = a(v, w), \quad \forall w \in W. \tag{3.32}$$

By Lax-Milgram theorem, P is well defined and $||Pv||_e \leq ||v||_e$. Let $\hat{\psi}_j = P\phi_j - \phi_j$. Then $\hat{\psi}_j \in \Psi_H$ since $P\hat{\psi}_j = 0$, $j = 1, \ldots, N_H$. And $\{\hat{\psi}_j\}_{j=1}^{N_H}$ spans Ψ_H since $\hat{\psi}_j$'s are linearly independent. Therefore

$$\psi_j = \sum_{k=1}^{N_H} \alpha_k^{(j)} (P\phi_k - \phi_k). \tag{3.33}$$

Note that $(\psi_j, \phi_\ell) = \delta_{j,\ell}$. Then $\sum_{k=1}^{N_H} \alpha_k^{(j)} (\phi_k, \phi_\ell) = -\delta_{j,\ell}$. So if we let $\alpha^{(j)} = (\alpha_1^{(j)}, \ldots, \alpha_{N_H}^{(j)})$, then $M\alpha^{(j)} = -e_j$, where e_j is a column vector with the j-th entry as 1 and other entries as 0 and M is the mass matrix with entries $M_{j,k} = (\phi_j, \phi_k)$.

From the results in [13, 14], $|(M^{-1})_{j,k}| \leq CH^{-d}$. Hence under Assumption 3.1, we have

$$||\nabla \psi_j|| \leq \sum_{k=1}^{N_H} \alpha_k^{(j)} ||\nabla (P\phi_k - \phi_k)|| \leq CN_H H^{-\frac{d}{2}} \leq CH^{-\frac{3}{2}d}. \tag{3.34}$$

□

We also need two lemmas on the difference between ψ_j and $\psi_j^{\text{loc},m}$.

Lemma 3.6. Under Assumption 3.1, for $j = 1, \ldots, N_H$

$$||\nabla (\psi_j - \psi_j^{\text{loc},m})|| \leq CH^{-\frac{3}{2}d} \beta^m. \tag{3.35}$$

Proof. Let $m \geq 6$ and $\tilde{\psi}_j = \psi_j - I_H^{-1,\text{loc}}(I_H \psi_j)$ and $\tilde{\psi}_j^{\text{loc},m} = \psi_j^{\text{loc},m} - I_H^{-1,\text{loc}}(I_H \psi_j^{\text{loc},m})$. Then $\psi_j - \psi_j^{\text{loc},m} = \tilde{\psi}_j - \tilde{\psi}_j^{\text{loc},m}$ since $I_H \psi_j = I_H \psi_j^{\text{loc},m} = \phi_j / (1, \phi_j)$. In addition, $\tilde{\psi}_j \in W$ and $\tilde{\psi}_j^{\text{loc},m} \in W(N^m(S_j))$. Then $\forall w \in W(N^m(S_j))$,

$$\begin{aligned} \varepsilon^2 ||\nabla (\tilde{\psi}_j - \tilde{\psi}_j^{\text{loc},m})||^2 &\leq a(\tilde{\psi}_j - \tilde{\psi}_j^{\text{loc},m}, \tilde{\psi}_j - \tilde{\psi}_j^{\text{loc},m}) = a(\tilde{\psi}_j - \tilde{\psi}_j^{\text{loc},m}, \tilde{\psi}_j - w) \\ &\leq ||\tilde{\psi}_j - \tilde{\psi}_j^{\text{loc},m}||_e ||\tilde{\psi}_j - w||_e \leq C\varepsilon^2 ||\nabla (\tilde{\psi}_j - \tilde{\psi}_j^{\text{loc},m})|| ||\nabla (\tilde{\psi}_j - w)||, \end{aligned} \tag{3.36}$$

where we have used the fact that $a(\psi_j, w - \tilde{\psi}_j^{\text{loc},m}) = a(\psi_j^{\text{loc},m}, w - \tilde{\psi}_j^{\text{loc},m}) = 0$ and hence $a(\tilde{\psi}_j - \tilde{\psi}_j^{\text{loc},m}, w - \tilde{\psi}_j^{\text{loc},m}) = a(\psi_j - \psi_j^{\text{loc},m}, w - \tilde{\psi}_j^{\text{loc},m}) = 0$.

Define the cutoff function

$$\eta = \frac{\text{dist}(\mathbf{x}, \Omega \backslash N^{m-2}(S_j))}{\text{dist}(\mathbf{x}, N^{m-3}(S_j)) + \text{dist}(\mathbf{x}, \Omega \backslash N^{m-2}(S_j))}. \tag{3.37}$$

Then $\eta = 1$ in $N^{m-3}(S_j)$, $\eta = 0$ in $\Omega \backslash N^{m-2}(S_j)$ and $0 \leq \eta \leq 1$ in $N^{m-2}(S_j) \backslash N^{m-3}(S_j)$. Furthermore, $H||\nabla \eta||_\infty \leq \gamma$ and $\text{supp}(\nabla \eta) = N^{m-2}(S_j) \backslash N^{m-3}(S_j)$.

Take $w = \eta \tilde{\psi}_j - I_H^{-1,\text{loc}}(I_H(\eta \tilde{\psi}_j)) \in W(N^m(S_j))$. Then

$$\begin{aligned}
||\nabla(\psi_j - \psi_j^{\text{loc},m})|| &= ||\nabla(\tilde{\psi}_j - \tilde{\psi}_j^{\text{loc},m})||^2 \leq C||\nabla(\tilde{\psi}_j - w)||^2 \leq C\varepsilon^{-2}||\tilde{\psi}_j - w||_e^2 \\
&\leq C\Big(||\nabla((1-\eta)\tilde{\psi}_j)||^2 + \frac{1}{\varepsilon^2}||(1-\eta)\tilde{\psi}_j||^2 \\
&+ ||\nabla(\eta\tilde{\psi}_j)||^2_{N^m(S_j)\backslash N^{m-5}(S_j)} + \frac{1}{\varepsilon^2}||\eta\tilde{\psi}_j||^2_{N^m(S_j)\backslash N^{m-5}(S_j)}\Big) \\
&\leq C\left(1 + \frac{H^2}{\varepsilon^2} + H^2||\nabla\eta||^2_\infty\right)||\nabla\psi_j||^2_{\Omega\backslash N^{m-5}(S_j)} + C\frac{H^2}{\varepsilon^2}||\nabla\psi_j||^2_{\Omega\backslash N^{m-6}(S_j)} \\
&\leq C||\nabla\psi_j||^2_{\Omega\backslash N^{m-6}(S_j)},
\end{aligned} \tag{3.38}$$

which completes the proof with Theorem 3.2 and Lemma 3.5. □

Lemma 3.7. Let $v \in H_P^1(\Omega)$ and $v_1 = \sum_{k=1}^{N_H}(v, \phi_k)\psi_k, v_2 = \sum_{k=1}^{N_H}(v, \phi_k)\psi_k^{\text{loc},m}$. Then under Assumption 3.1, we have

$$||v_1 - v_2||_e \leq C\varepsilon H^{-\frac{3}{2}d}\beta^m||v||_e. \tag{3.39}$$

Proof. Note that $v_1 - v_2 \in W$. Then

$$\begin{aligned}
||v_1 - v_2||_e \leq C\varepsilon||\nabla(v_1 - v_2)|| &\leq C\varepsilon\sum_{k=1}^{N_H}|(v, \phi_k)|||\nabla(\psi_k - \psi_k^{\text{loc},m})|| \\
&\leq C\varepsilon H^{-\frac{3}{2}d}\beta^m(|v|, 1) \leq C\varepsilon H^{-\frac{3}{2}d}\beta^m||v||_e.
\end{aligned} \tag{3.40}$$

□

Similarly, the Galerkin approximation of (2.5) in $\Psi_{H,m}$ is to seek $u_{H,m} \in \Psi_{H,m}$ such that

$$a(u_{H,m}, v_{H,m}) = (f, v_{H,m}), \quad \forall v_{H,m} \in \Psi_{H,m}. \tag{3.41}$$

In order to obtain the projection error estimate for the localized multiscale finite element space $\Psi_{H,m}$, we need the following assumption on the oversampling size m.

Assumption 3.2. The oversamping size m satisfies

$$m \geq \frac{C_d \log(1/H) + \log(\varepsilon^2 C_{\text{st}}(\varepsilon, V))}{|\log(\beta)|}, \tag{3.42}$$

where $C_d = 3d/2 + 2$.

Then we have an error estimate for $u - u_{H,m}$.

Theorem 3.3. Assume that Assumptions 3.1 and 3.2 hold and let u the solution of (2.5) and $u_{H,m}$ be the solution of (3.41). If $f \in L^2(\Omega)$, then

$$||u - u_{H,m}||_e \leq C\frac{H}{\varepsilon}||f||, \tag{3.43}$$

$$||u - u_{H,m}|| \leq C\frac{H^2}{\varepsilon^2}||f||. \tag{3.44}$$

Moreover, If $f \in H^1(\Omega)$, then

$$||u - u_{H,m}||_e \leq C\frac{H^2}{\varepsilon}||f||_{H^1}, \tag{3.45}$$

$$||u - u_{H,m}|| \leq C\frac{H^3}{\varepsilon^2}||f||_{H^1}. \tag{3.46}$$

Proof. We first consider the case where $f \in L^2(\Omega)$. Let $\tilde{u}_{H,m} = \sum_{k=1}^{N_H}(u, \phi_k)\psi_k^{\text{loc},m}$. Then it is easy to verify that

$$||u - u_{H,m}||_e \leq ||u - \tilde{u}_{H,m}||_e. \tag{3.47}$$

Set $u_H = \sum_{k=1}^{N_H}(u, \phi_k)\psi_k$. Then since $u - \tilde{u}_{H,m} \in W$, $a(u_H, u - \tilde{u}_{H,m}) = 0$ and

$$\begin{aligned}
||u - \tilde{u}_{H,m}||_e^2 &= a(u - \tilde{u}_{H,m}, u - \tilde{u}_{H,m}) = a(u, u - \tilde{u}_{H,m}) + a(u_H - \tilde{u}_{H,m}, u - \tilde{u}_{H,m}) \\
&= (f, u - \tilde{u}_{H,m}) + a(u_H - \tilde{u}_{H,m}, u - \tilde{u}_{H,m}) \\
&\leq CH||f||||\nabla(u - \tilde{u}_{H,m})|| + ||u_H - \tilde{u}_{H,m}||_e||u - \tilde{u}_{H,m}||_e \\
&\leq C\frac{H}{\varepsilon}||f||||u - \tilde{u}_{H,m}||_e + C\varepsilon H^{-\frac{3}{2}d}\beta^m||u||_e||u - \tilde{u}_{H,m}||_e \\
&\leq C\frac{H}{\varepsilon}||f||||u - \tilde{u}_{H,m}||_e + C\varepsilon H^{-\frac{3}{2}d}C_{\text{st}}(\varepsilon, V)\beta^m||f||||u - \tilde{u}_{H,m}||_e.
\end{aligned} \tag{3.48}$$

Hence if m satisfies Assumption 3.2, then

$$||u - u_{H,m}||_e \leq C\frac{H}{\varepsilon}||f||. \tag{3.49}$$

A similar Aubin-Nitsche technique to the proof of Theorem 3.1 can be applied to obtain (3.44).

Moreover, if $f \in H^1(\Omega)$, we have by Lemma 2.5 that

$$\begin{aligned}
||u - \tilde{u}_{H,m}||_e^2 &= (f, u - \tilde{u}_{H,m}) + a(u_H - \tilde{u}_{H,m}, u - \tilde{u}_{H,m}) \\
&\leq C\frac{H^2}{\varepsilon}||\nabla f||||u - \tilde{u}_{H,m}||_e + C\varepsilon H^{-\frac{3}{2}d}C_{\text{st}}(\varepsilon, V)\beta^m||f||||u - \tilde{u}_{H,m}||_e.
\end{aligned} \tag{3.50}$$

Hence if m satisfies Assumption 3.2, we can obtain

$$||u - u_{H,m}||_e \leq C\frac{H^2}{\varepsilon}||f||_{H^1}. \tag{3.51}$$

Analogously, we obtain (3.46) using the Aubin-Nitsche technique. □

Remark 3.1. To obtain (3.43) and (3.44), it is sufficient to assume that m satisfies (3.42) with $C_d = 3d/2 + 1$. We impose a stronger assumption on m in order to avoid lengthy illustration of Theorem 3.3.

4. Convergence of the OC MsFEM for Schrödinger equations with multiscale potentials

In this section, we will study the error estimate of the Galerkin approximation obtained by the OC MsFEM for the Schrödinger equation (2.1). Throughout this section, we will not distinguish between the global multiscale finite element space Ψ_H and the localized multiscale finite element space $\Psi_{H,m}$ with H satisfying Assumption 3.1 and m satisfying Assumption 3.2. Both of the spaces will be denoted by Ψ_H.

4.1. Projection error

Let $u(t)$ be the solution of the Schrödinger equation (2.1) and $\hat{u}(t)$ be the projection of $u(t)$ in Ψ_H such that $\forall 0 \le t \le T, \hat{u}(t) \in \Psi_H$ and

$$a(u(t) - \hat{u}(t), w) = 0, \quad \forall w \in \Psi_H. \tag{4.1}$$

Then, we have the following lemmas on the projection errors.

Lemma 4.1. If $u_t(t) \in L^2(\Omega)$ for any $t \in [0, T]$, then it holds true for any $0 \le t \le T$ that

$$||u(t) - \hat{u}(t)||_e \le C\frac{H}{\varepsilon}, \quad \text{and}, \quad ||u(t) - \hat{u}(t)|| \le C\frac{H^2}{\varepsilon^2}. \tag{4.2}$$

Moreover, if $u_t(t) \in H^1(\Omega)$ for any $t \in [0, T]$, then it holds true for any $0 \le t \le T$ that

$$||u(t) - \hat{u}(t)||_e \le C\frac{H^2}{\varepsilon^2 \delta}, \quad \text{and}, \quad ||u(t) - \hat{u}(t)|| \le C\frac{H^3}{\varepsilon^3 \delta}. \tag{4.3}$$

Proof. We first consider the case where $u_t(t) \in L^2(\Omega), \forall t \in [0, T]$. By (2.1), Theorems 3.1, 3.3 and Lemma 2.2, we have that for any $0 \le t \le T$,

$$||u(t) - \hat{u}(t)||_e \le C\frac{H}{\varepsilon}||\mathcal{H}u(t)|| \le CH||u_t(t)|| \le C\frac{H}{\varepsilon}, \tag{4.4}$$

$$||u(t) - \hat{u}(t)|| \le C\frac{H^2}{\varepsilon^2}||\mathcal{H}u(t)|| \le C\frac{H^2}{\varepsilon}||u_t(t)|| \le C\frac{H^2}{\varepsilon^2}. \tag{4.5}$$

Moreover, if $u_t(t) \in H^1(\Omega)$ for any $t \in [0, T]$, by (2.1), Theorems 3.1, 3.3 and Lemmas 2.2, 2.4, for any $0 \le t \le T$,

$$||u(t) - \hat{u}(t)||_e \le C\frac{H^2}{\varepsilon}||\mathcal{H}u(t)||_{H^1} \le CH^2||u_t(t)||_{H^1} \le C\frac{H^2}{\varepsilon^2 \delta}, \tag{4.6}$$

$$||u(t) - \hat{u}(t)|| \le C\frac{H^3}{\varepsilon^2}||\mathcal{H}u(t)||_{H^1} \le C\frac{H^3}{\varepsilon}||u_t(t)||_{H^1} \le C\frac{H^3}{\varepsilon^3 \delta}. \tag{4.7}$$

□

Lemma 4.2. If $\partial_t^{k+1} u(t) \in L^2(\Omega)$ for any $t \in [0, T]$ and $k = 1, 2$, then it holds true for any $0 \le t \le T$ that

$$||\partial_t^k u(t) - \partial_t^k \hat{u}(t)||_e \le \frac{CH}{\varepsilon^{1-k} \min\{\varepsilon^{2k}, \delta^{2k}\}}, \quad ||\partial_t^k u(t) - \partial_t^k \hat{u}(t)|| \le \frac{CH^2}{\varepsilon^{2-k} \min\{\varepsilon^{2k}, \delta^{2k}\}}. \tag{4.8}$$

Moreover, if $\partial_t^{k+1} u(t) \in H^1(\Omega)$ for any $t \in [0,T]$ and $k = 1,2$, then it holds true for any $0 \le t \le T$ that

$$||\partial_t^k u(t) - \partial_t^k \hat{u}(t)||_e \le \frac{CH^2}{\varepsilon^{2-k}\delta \min\{\varepsilon^{2k}, \delta^{2k}\}}, \quad ||\partial_t^k u(t) - \partial_t^k \hat{u}(t)|| \le \frac{CH^3}{\varepsilon^{3-k}\delta \min\{\varepsilon^{2k}, \delta^{2k}\}}. \quad (4.9)$$

The proof of Lemma 4.2 is similar to that of Lemma 4.1. It can be easily seen that higher regularity of the solution u will lead to super-convergence of the projection errors in Ψ_H w.r.t. H.

We can also study the error of the finite element method in solving the Schrödinger equation (2.1). Let $\tilde{u}$ be the projection of u in the standard linear finite element space Φ_H such that $\forall 0 \le t \le T$, $\tilde{u} \in \Phi_H$ and

$$a(u(t) - \tilde{u}(t), w) = 0, \quad \forall w \in \Phi_H. \quad (4.10)$$

Then

$$||u(t) - \tilde{u}(t)||_e \le \inf_{w \in \Phi_H} ||u(t) - w||_e. \quad (4.11)$$

Let $\chi(t)$ be the interpolation of $u(t)$ in Φ_H such that $\chi = \sum_{\mathbf{x}_k \in \mathcal{N}_H} u(t, \mathbf{x}_k)\phi_k$, where $\phi_j(\mathbf{x}_k) = \delta_{j,k}$. A well known result for the errors of the interpolation [2, 6, 41] is that

$$||\chi(t) - u(t)|| \le CH^2 ||u(t)||_{H^2}, \text{ and }, ||\nabla(\chi(t) - u(t))|| \le CH||u(t)||_{H^2} \quad (4.12)$$

and hence

$$||u(t) - \tilde{u}(t)||_e \le ||\chi(t) - u(t)||_e \le C\varepsilon H \sqrt{1 + \frac{H^2}{\varepsilon^2}} ||u(t)||_{H^2}. \quad (4.13)$$

By Lemma 2.3 and under Assumption 3.1, we know that for any $0 \le t \le T$,

$$||u(t) - \tilde{u}(t)||_e \le C \frac{H}{\varepsilon \delta^2}. \quad (4.14)$$

Using the Aubin-Nitsche technique with H^2 regularity of elliptic equations [12, 14], we obtain that for any $0 \le t \le T$,

$$||u(t) - \tilde{u}(t)|| \le CH^2 ||u||_{H^2} \le C \frac{H^2}{\varepsilon^2 \delta^2}. \quad (4.15)$$

In comparison with Lemma 4.1, we find that the error analysis of FEM depends on higher spatial regularity of the solution u. In the presence of the multiscale potential V^δ, the spatial derivatives of u become more oscillatory than the time derivatives of u. Therefore, using the same mesh size the OC MsFEM gives more accurate results than FEM in solving Schrödinger equation with multiscale potentials due to its super convergence behavior and weaker dependence on the small parameters ε and δ.

4.2. Semi-discrete approximations

Let $u_H(t)$ be the Galerkin approximation in Ψ_H for the solution u of the Schrödinger equation (2.1) such that $u_H(t) \in \Psi_H$ for any $0 \le t \le T$ and

$$\begin{aligned} i\varepsilon(u_{H,t}, w) &= a(u_H, w), \quad \forall w \in \Psi_H, 0 \le t \le T, \\ u_H(0) &= \hat{u}(0), \end{aligned} \quad (4.16)$$

where $u_{H,t} = \partial_t u_H$. Then for the initial value $u_H(0)$, we have the following estimate.

Lemma 4.3. Assume that $u_{tt}(0) \in L^2(\Omega)$. Then

$$||u_{H,t}(0) - \hat{u}_t(0)|| \leq \frac{CH^2}{\varepsilon \min\{\varepsilon^2, \delta^2\}}. \tag{4.17}$$

Moreover, if $u_{tt}(0) \in H^1(\Omega)$, then

$$||u_{H,t}(0) - \hat{u}_t(0)|| \leq \frac{CH^3}{\varepsilon^2 \delta \min\{\varepsilon^2, \delta^2\}}. \tag{4.18}$$

Proof. For any $w \in \Psi_H$,

$$i\varepsilon(u_{H,t}(0), w) = a(u_H(0), w) = a(\hat{u}(0), w) = a(u_0, w) = i\varepsilon(u_t(0), w). \tag{4.19}$$

Taking $w = u_{H,t}(0) - \hat{u}_t(0)$, we have $(u_{H,t}(0) - u_t(0), u_{H,t}(0) - \hat{u}_t(0)) = 0$. Hence

$$||u_{H,t}(0) - \hat{u}_t(0)||^2 \leq ||u_t(0) - \hat{u}_t(0)||||u_{H,t}(0) - \hat{u}_t(0)||. \tag{4.20}$$

If $u_{tt}(0) \in L^2(\Omega)$, $||u_t(0) - \hat{u}_t(0)|| \leq C\frac{H^2}{\varepsilon}||u_{tt}(0)|| \leq \frac{CH^2}{\varepsilon \min\{\varepsilon^2, \delta^2\}}$. Moreover, if $u_{tt}(0) \in H^1(\Omega)$, $||u_t(0) - \hat{u}_t(0)|| \leq C\frac{H^3}{\varepsilon}||u_{tt}(0)||_{H^1} \leq \frac{CH^3}{\varepsilon^2 \delta \min\{\varepsilon^2, \delta^2\}}$. And the proof is completed. □

Let $u_H - u = \theta + \rho$, where $\theta = u_H - \hat{u}$ and $\rho = \hat{u} - u$. Then

$$i\varepsilon(\theta_t, w) + i\varepsilon(\rho_t, w) = a(\theta, w) + a(\rho, w) = a(\theta, w), \quad \forall w \in \Psi_H. \tag{4.21}$$

Take $w = \theta$ and we have

$$i\varepsilon(\theta_t, \theta) + i\varepsilon(\rho_t, \theta) = a(\theta, \theta). \tag{4.22}$$

We first estimate the L^2 error $||u_H(T) - u(T)||$.

Theorem 4.1. Assume that u is the solution of (2.1) and u_H is the solution of (4.16). If $u_t(t), u_{tt}(t) \in L^2(\Omega)$ for any $t \in [0, T]$, then

$$||u_H(T) - u(T)|| \leq \frac{CH^2}{\varepsilon \min\{\varepsilon^2, \delta^2\}}. \tag{4.23}$$

Moreover, if $u_t(t), u_{tt}(t) \in H^1(\Omega)$ for any $t \in [0, T]$, then

$$||u_H(T) - u(T)|| \leq \frac{CH^3}{\varepsilon^2 \delta \min\{\varepsilon^2, \delta^2\}}. \tag{4.24}$$

Proof. we first consider the case where $u_t(t), u_{tt}(t) \in L^2(\Omega), \forall t \in [0, T]$. Note that $||u_H - u|| \leq ||\theta|| + ||\rho||$ and $||\rho(T)|| \leq C\frac{H^2}{\varepsilon}||u_t(T)|| \leq C\frac{H^2}{\varepsilon^2}$, $\theta(0) = 0$. Take the imaginary part of (4.22) and we have $\mathrm{Re}(\theta_t, \theta) = -\mathrm{Re}(\rho_t, \theta)$, which implies

$$\frac{1}{2}\frac{d}{dt}||\theta||^2 = ||\theta||\frac{d}{dt}||\theta|| \leq ||\rho_t||||\theta||. \tag{4.25}$$

And hence for any $0 \leq t \leq T$, we obtain

$$\frac{d}{dt}||\theta(t)|| \leq ||\rho_t(t)|| \leq C\frac{H^2}{\varepsilon}||u_{tt}(t)|| \leq \frac{CH^2}{\varepsilon \min\{\varepsilon^2, \delta^2\}}. \tag{4.26}$$

The above estimate (4.26) implies that $||\theta(T)|| \le \frac{CH^2}{\varepsilon\min\{\varepsilon^2,\delta^2\}}$. Therefore, we can get that

$$||u_H(T) - u(T)|| \le \frac{CH^2}{\varepsilon\min\{\varepsilon^2,\delta^2\}}. \tag{4.27}$$

Moreover, if $u_t(t), u_{tt}(t) \in H^1(\Omega)$ for any $t \in [0, T]$, then

$$||\rho(T)|| \le C\frac{H^3}{\varepsilon}||u_t(T)||_{H^1} \le C\frac{H^3}{\varepsilon^3\delta} \tag{4.28}$$

and for any $0 \le t \le T$,

$$||\rho_t(t)|| \le C\frac{H^3}{\varepsilon}||u_{tt}(t)||_{H^1} \le \frac{CH^3}{\varepsilon^2\delta\min\{\varepsilon^2,\delta^2\}}. \tag{4.29}$$

And we can obtain (4.24) using similar arguments. □

Similarly, we can estimate the error in the energy norm.

Theorem 4.2. Assume that u is the solution of (2.1) and u_H is the solution of (4.16). If $u_t(t), u_{tt}(t), u_{ttt}(t) \in L^2(\Omega)$ for any $t \in [0, T]$, then

$$||u_H(T) - u(T)||_e \le C\left(\frac{H}{\varepsilon} + \frac{H^2}{\min\{\varepsilon^3,\delta^3\}}\right). \tag{4.30}$$

Moreover, if $u_t(t), u_{tt}(t), u_{ttt}(t) \in H^1(\Omega)$ for any $t \in [0, T]$, then

$$||u_H(T) - u(T)||_e \le C\left(\frac{H^2}{\varepsilon^2\delta} + \frac{H^3}{\varepsilon\delta\min\{\varepsilon^3,\delta^3\}}\right). \tag{4.31}$$

Proof. First consider the case where $u_t(t), u_{tt}(t), u_{ttt}(t) \in L^2(\Omega), \forall t \in [0, T]$. We have $||u_H - u||_e \le ||\theta||_e + ||\rho||_e$ and $||\rho(T)||_e \le CH||u_t(T)|| \le C\frac{H}{\varepsilon}, \theta(0) = 0$. Then, by (4.22), we have

$$||\theta||_e^2 = a(\theta,\theta) \le \varepsilon(|(\theta_t,\theta)| + |(\rho_t,\theta)|) \le \varepsilon||\theta||(||\theta_t|| + ||\rho_t||). \tag{4.32}$$

For $||\theta||$, we have from Theorem 4.1 that $||\theta(T)|| \le \frac{CH^2}{\varepsilon\min\{\varepsilon^2,\delta^2\}}$. For $||\rho_t||$, we have $||\rho_t(T)|| \le C\frac{H^2}{\varepsilon}||u_{tt}(T)|| \le \frac{CH^2}{\varepsilon\min\{\varepsilon^2,\delta^2\}}$. For $||\theta_t||$, similarly to the derivation of (4.22), we can derive that

$$i\varepsilon(\theta_{tt},\theta_t) + i\varepsilon(\rho_{tt},\theta_t) = a(\theta_t,\theta_t). \tag{4.33}$$

By taking the imaginary part, we will obtain

$$\frac{d}{dt}||\theta_t(t)|| \le ||\rho_{tt}(t)|| \le C\frac{H^2}{\varepsilon}||u_{ttt}(t)|| \le \frac{CH^2}{\min\{\varepsilon^4,\delta^4\}}, \quad \forall t \in [0, T]. \tag{4.34}$$

Hence by Lemma 4.3,

$$||\theta_t(T)|| \le ||\theta_t(0)|| + \frac{CH^2}{\min\{\varepsilon^4,\delta^4\}} \le \frac{CH^2}{\min\{\varepsilon^4,\delta^4\}}. \tag{4.35}$$

Combining all the above inequalities, we obtain

$$||u_H(T) - u(T)||_e \le C\left(\frac{H}{\varepsilon} + \frac{H^2}{\min\{\varepsilon^3, \delta^3\}}\right). \tag{4.36}$$

Moreover, if $u_t(t), u_{tt}(t), u_{ttt}(t) \in H^1(\Omega)$ for any $t \in [0, T]$, we have

$$||\theta_t(0)|| \le \frac{CH^3}{\varepsilon^2\delta\min\{\varepsilon^2, \delta^2\}}, \quad ||\rho(T)||_e \le CH^2||u_t(T)||_{H^1} \le C\frac{H^2}{\varepsilon^2\delta}, \tag{4.37}$$

$$||\theta(T)|| \le \frac{CH^3}{\varepsilon^2\delta\min\{\varepsilon^2, \delta^2\}}, \quad ||\rho_t(T)|| \le C\frac{H^3}{\varepsilon}||u_{tt}(T)||_{H^1} \le \frac{CH^3}{\varepsilon^2\delta\min\{\varepsilon^2, \delta^2\}}, \tag{4.38}$$

and for any $0 \le t \le T$,

$$||\rho_{tt}(t)|| \le C\frac{H^3}{\varepsilon}||u_{ttt}(t)||_{H^1} \le \frac{CH^3}{\varepsilon\delta\min\{\varepsilon^4.\delta^4\}}. \tag{4.39}$$

The statment in (4.31) can be obtained by using similar arguments. □

4.3. Fully discrete approximations

In this subsection, we discuss the backward Euler scheme and the Crank-Nicolson scheme in temporal discretization. Combining the spatial discretization using the OC MsFEM, we obtain the fully discrete Galerkin approximation for the Schrödinger equation (2.1). And we focus on the error estimates of the numerical solutions obtained by such fully discrete schemes. In what follows, we introduce some notations. For some $N \in \mathbb{N}$ and $N > 0$, let $\Delta t = \frac{T}{N}$ and $t_n = n\Delta t, n = 0, 1, \ldots, N$.

4.3.1. Backward Euler scheme

Using the backward Euler scheme, we approximate $u(t_n)$ by $U^n \in \Psi_H$ such that

$$\begin{aligned} i\varepsilon(\bar{\partial}U^n, w) &= a(U^n, w), \quad \forall w \in \Psi_H, n = 1, \ldots, N, \\ U^0 &= \hat{u}(0), \end{aligned} \tag{4.40}$$

where $\bar{\partial}U^n = \frac{U^n - U^{n-1}}{\Delta t}$. Let $U^n - u(t_n) = \theta^n + \rho^n$, where $\theta^n = U^n - \hat{u}(t_n)$ and $\rho^n = \hat{u}(t_n) - u(t_n)$. Then θ^n satisfies that $\theta^0 = 0$ and

$$i\varepsilon(\bar{\partial}\theta^n, w) + i\varepsilon(\bar{\partial}\hat{u}(t_n) - u_t(t_n), w) = a(\theta^n, w) + a(\rho^n, w) = a(\theta^n, w), \quad \forall w \in \Psi_H, n = 1, \ldots, N, \tag{4.41}$$

where $\bar{\partial}\hat{u}(t_n) = \frac{\hat{u}(t_n) - \hat{u}(t_{n-1})}{\Delta t}$. Taking $w = \theta^n$, we have

$$i\varepsilon(\bar{\partial}\theta^n, \theta^n) + i\varepsilon(z_1^n, \theta^n) + i\varepsilon(z_2^n, \theta^n) = a(\theta^n, \theta^n), \quad n = 1, \ldots, N, \tag{4.42}$$

where $z_1^n = \bar{\partial}\hat{u}(t_n) - \bar{\partial}u(t_n)$ and $z_2^n = \bar{\partial}u(t_n) - u_t(t_n)$ with $\bar{\partial}u(t_n) = \frac{u(t_n) - u(t_{n-1})}{\Delta t}$.

For the L^2 error, we have the following theorem.

Theorem 4.3. Assume that U^N is the solution of (4.40) and u is the solution of (2.1). If $u_t(t), u_{tt}(t) \in L^2(\Omega)$ for any $t \in [0,T]$, then

$$||U^N - u(T)|| \leq C\left(\frac{\Delta t}{\min\{\varepsilon^2, \delta^2\}} + \frac{H^2}{\varepsilon \min\{\varepsilon^2, \delta^2\}}\right). \tag{4.43}$$

Moreover, if $u_t(t), u_{tt}(t) \in H^1(\Omega)$ for any $t \in [0,T]$, then

$$||U^N - u(T)|| \leq C\left(\frac{\Delta t}{\min\{\varepsilon^2, \delta^2\}} + \frac{H^3}{\varepsilon^2\delta \min\{\varepsilon^2, \delta^2\}}\right). \tag{4.44}$$

Proof. We first consider the case where $u_t(t), u_{tt}(t) \in L^2(\Omega), \forall t \in [0,T]$. We have $||U^n - u(t_n)|| \leq ||\theta^n|| + ||\rho^n||$ and $||\rho^N|| \leq C\frac{H^2}{\varepsilon}||u_t(T)|| \leq C\frac{H^2}{\varepsilon^2}$. For θ^n, taking the imaginary part of (4.42), we have

$$(\theta^n, \theta^n) = (\theta^{n-1}, \theta^n) - \Delta t\big((z_1^n, \theta^n) + (z_2^n, \theta^n)\big). \tag{4.45}$$

Hence, we obtain $||\theta^n||^2 \leq ||\theta^n||||\theta^{n-1}|| + \Delta t||\theta^n||(||z_1^n|| + ||z_2^n||)$, which implies

$$||\theta^N|| \leq ||\theta^0|| + \Delta t\sum_{n=1}^{N}(||z_1^n|| + ||z_2^n||) = \Delta t\sum_{n=1}^{N}(||z_1^n|| + ||z_2^n||). \tag{4.46}$$

On one hand, we know that for $n = 1, 2, \ldots, N$,

$$\begin{aligned}||z_1^n|| = ||\bar{\partial}\hat{u}(t_n) - \bar{\partial}u(t_n)|| &\leq \frac{1}{\Delta t}\int_{t_{n-1}}^{t_n} ||\hat{u}_t(s) - u_t(s)||ds \\ &\leq \frac{C}{\Delta t}\frac{H^2}{\varepsilon}\int_{t_{n-1}}^{t_n} ||u_{tt}(s)||ds \leq \frac{CH^2}{\varepsilon\min\{\varepsilon^2, \delta^2\}}.\end{aligned} \tag{4.47}$$

This gives us that $\Delta t\sum_{n=1}^{N}||z_1^n|| \leq \frac{CH^2}{\varepsilon\min\{\varepsilon^2,\delta^2\}}$. On the other hand, we have for $n = 1, 2, \ldots, N$,

$$||z_2^n|| \leq \frac{1}{\Delta t}\int_{t_{n-1}}^{t_n} ||(s - t_{n-1})u_{tt}(s)||ds \leq \int_{t_{n-1}}^{t_n} ||u_{tt}(s)||ds \leq \frac{C\Delta t}{\min\{\varepsilon^2, \delta^2\}}. \tag{4.48}$$

This gives us that $\Delta t\sum_{n=1}^{N}||z_2^n|| \leq \frac{C\Delta t}{\min\{\varepsilon^2,\delta^2\}}$. Therefore, we obtain

$$||\theta^N|| \leq C\left(\frac{\Delta t}{\min\{\varepsilon^2, \delta^2\}} + \frac{H^2}{\varepsilon\min\{\varepsilon^2, \delta^2\}}\right) \tag{4.49}$$

and hence

$$||U^N - u(T)|| \leq C\left(\frac{\Delta t}{\min\{\varepsilon^2, \delta^2\}} + \frac{H^2}{\varepsilon\min\{\varepsilon^2, \delta^2\}}\right). \tag{4.50}$$

Moreover, if $u_t(t), u_{tt}(t) \in H^1(\Omega)$ for any $t \in [0,T]$, then we have

$$||\rho^N|| \leq C\frac{H^3}{\varepsilon}||u_t(T)||_{H^1} \leq C\frac{H^3}{\varepsilon^3\delta} \tag{4.51}$$

and for $n = 1, 2, \ldots, N$,

$$||z_1^n|| \leq \frac{C}{\Delta t}\frac{H^3}{\varepsilon}\int_{t_{n-1}}^{t_n} ||u_{tt}(s)||_{H^1}ds \leq \frac{CH^3}{\varepsilon^2\delta\min\{\varepsilon^2, \delta^2\}}. \tag{4.52}$$

Finally, we can prove (4.44) using similar arguments. □

We can also obtain the error estimate in the energy norm as stated in the following theorem.

Theorem 4.4. Assume that U^N is the solution of (4.40) and u is the solution of (2.1). If $u_t(t), u_{tt}(t), u_{ttt}(t) \in L^2(\Omega)$ for any $t \in [0,T]$, then

$$||U^N - u(T)||_e \le C\left(\frac{H}{\varepsilon} + \frac{H^2}{\min\{\varepsilon^3, \delta^3\}} + \frac{\varepsilon\Delta t}{\min\{\varepsilon^3, \delta^3\}}\right). \tag{4.53}$$

Moreover, if $u_t(t), u_{tt}(t), u_{ttt}(t) \in H^1(\Omega)$ for any $t \in [0,T]$, then

$$||U^N - u(T)||_e \le C\left(\frac{H^2}{\varepsilon^2\delta} + \frac{H^3}{\varepsilon\delta\min\{\varepsilon^3, \delta^3\}} + \frac{\varepsilon\Delta t}{\min\{\varepsilon^3, \delta^3\}}\right). \tag{4.54}$$

Proof. First consider the case where $u_t(t), u_{tt}(t), u_{ttt}(t) \in L^2(\Omega), \forall t \in [0,T]$. We have $||U^n - u(t_n)||_e \le ||\theta^n||_e + ||\rho^n||_e$ and $||\rho^N||_e \le CH||u_t(T)|| \le C\frac{H}{\varepsilon}$. By (4.42), we have

$$||\theta^n||_e^2 = a(\theta^n, \theta^n) \le \varepsilon(|(\bar\partial\theta^n, \theta^n)| + |(z_1^n, \theta^n)| + |(z_2^n, \theta^n)|) \le \varepsilon||\theta^n||(||\bar\partial\theta^n|| + ||z_1^n|| + ||z_2^n||). \tag{4.55}$$

From the proof of Theorem 4.3,

$$||\theta^N|| \le C\left(\frac{\Delta t}{\min\{\varepsilon^2, \delta^2\}} + \frac{H^2}{\varepsilon\min\{\varepsilon^2, \delta^2\}}\right), \quad ||z_1^N|| \le \frac{CH^2}{\varepsilon\min\{\varepsilon^2, \delta^2\}}, \quad ||z_2^N|| \le \frac{C\Delta t}{\min\{\varepsilon^2, \delta^2\}}.$$

For $||\bar\partial\theta^n||$, in a similar way to derive (4.42), we can derive that

$$i\varepsilon(\bar\partial(\theta^n - \theta^{n-1}), \bar\partial\theta^n) + i\varepsilon(z_1^n - z_1^{n-1}, \bar\partial\theta^n) + i\varepsilon(z_2^n - z_2^{n-1}, \bar\partial\theta^n) = a(\theta^n - \theta^{n-1}, \bar\partial\theta^n). \tag{4.56}$$

Taking the imaginary part of this equation and we can obtain

$$\begin{aligned} ||\bar\partial\theta^n||^2 = (\bar\partial\theta^n, \bar\partial\theta^n) &\le |(\bar\partial\theta^{n-1}, \bar\partial\theta^n)| + |(z_1^n - z_1^{n-1}, \bar\partial\theta^n)| + |(z_2^n - z_2^{n-1}, \bar\partial\theta^n)| \\ &\le ||\bar\partial\theta^n||(||\bar\partial\theta^{n-1}|| + ||z_1^n - z_1^{n-1}|| + ||z_2^n - z_2^{n-1}||). \end{aligned} \tag{4.57}$$

And hence

$$||\bar\partial\theta^N|| \le ||\bar\partial\theta^1|| + \sum_{n=2}^{N}(||z_1^n - z_1^{n-1}|| + ||z_2^n - z_2^{n-1}||). \tag{4.58}$$

For $||\bar\partial\theta^1||$, from the proof of Theorem 4.3, we have

$$||\bar\partial\theta^1|| = \frac{1}{\Delta t}||\theta^1 - \theta^0|| \le \frac{1}{\Delta t}||\theta^1|| \le ||z_1^1|| + ||z_2^1|| \le C\left(\frac{H^2}{\varepsilon\min\{\varepsilon^2, \delta^2\}} + \frac{\Delta t}{\min\{\varepsilon^2, \delta^2\}}\right). \tag{4.59}$$

For $||z_1^n - z_1^{n-1}||$, $n = 2, 3, \dots, N$, we have

$$\begin{aligned} ||z_1^n - z_1^{n-1}|| &= \frac{1}{\Delta t}||\rho(t_n) - 2\rho(t_{n-1}) + \rho(t_{n-2})|| \\ &\le \frac{1}{\Delta t}\left(\int_{t_{n-1}}^{t_n}(t_n - s)||\rho_{tt}(s)||ds + \int_{t_{n-2}}^{t_{n-1}}(s - t_{n-2})||\rho_{tt}(s)||ds\right) \\ &\le C\frac{\Delta t H^2}{\varepsilon}\max_{0\le t\le T}||u_{ttt}(t)|| \le \frac{C\Delta t H^2}{\min\{\varepsilon^4, \delta^4\}} \end{aligned} \tag{4.60}$$

and hence $\sum_{n=2}^{N}||z_1^n - z_1^{n-1}|| \leq \frac{CH^2}{\min\{\varepsilon^4,\delta^4\}}$. For the terms $||z_2^n - z_2^{n-1}||$, $n = 2, 3, \ldots, N$, we have

$$\begin{aligned}
||z_2^n - z_2^{n-1}|| &= \frac{1}{\Delta t}||(u(t_n) - 2u(t_{n-1}) + u(t_{n-2})) - \Delta t(u_t(t_n) - u_t(t_{n-1}))|| \\
&\leq \frac{1}{2\Delta t}\Big(\int_{t_{n-1}}^{t_n}(t_n - s)^2||u_{ttt}(s)||ds + \int_{t_{n-2}}^{t_{n-1}}(s - t_{n-2})^2||u_{ttt}(s)||ds \\
&+ 2\Delta t\int_{t_{n-1}}^{t_n}(t_n - s)||u_{ttt}(s)||ds\Big) \\
&\leq C\Delta t^2 \max_{0\leq t\leq T}||u_{ttt}(t)|| \leq \frac{C\varepsilon\Delta t^2}{\min\{\varepsilon^4, \delta^4\}}
\end{aligned} \tag{4.61}$$

and hence $\sum_{n=2}^{N}||z_2^n - z_2^{n-1}|| \leq \frac{C\varepsilon\Delta t}{\min\{\varepsilon^4,\delta^4\}}$. Combining all the above inequalities, we obtain that

$$||U^N - u(T)||_e \leq C\left(\frac{H}{\varepsilon} + \frac{H^2}{\min\{\varepsilon^3, \delta^3\}} + \frac{\varepsilon\Delta t}{\min\{\varepsilon^3, \delta^3\}}\right). \tag{4.62}$$

Moreover, if $u_t(t), u_{tt}(t), u_{ttt}(t) \in H^1(\Omega)$ for any $t \in [0, T]$, then we have

$$||\rho^N||_e \leq CH^2||u_t(T)||_{H^1} \leq C\frac{H^2}{\varepsilon^2\delta} \tag{4.63}$$

and for $n = 2, 3, \ldots, N$,

$$||z_1^n - z_1^{n-1}|| \leq C\frac{\Delta t H^3}{\varepsilon}\max_{0\leq t\leq T}||u_{ttt}(t)||_{H^1} \leq \frac{C\Delta t H^3}{\varepsilon\delta\min\{\varepsilon^4, \delta^4\}}. \tag{4.64}$$

And from the proof of Theorem 4.3, we already know that $||\theta^N|| \leq C\left(\frac{\Delta t}{\min\{\varepsilon^2,\delta^2\}} + \frac{H^3}{\varepsilon^2\delta\min\{\varepsilon^2,\delta^2\}}\right)$ and for $n = 1, 2, \ldots, N$, $||z_1^n|| \leq \frac{CH^3}{\varepsilon^2\delta\min\{\varepsilon^2,\delta^2\}}$. Hence we can prove (4.54) using similar arguments. □

4.3.2. Crank-Nicolson scheme

Using the Crank-Nicolson scheme, we approximate $u(t_n)$ by $U^n \in \Psi_H$ such that

$$\begin{aligned}
i\varepsilon(\bar{\partial}U^n, w) &= a\left(\frac{U^n + U^{n-1}}{2}, w\right), \quad \forall w \in \Psi_H, n = 1, \ldots, N, \\
U^0 &= \hat{u}(0).
\end{aligned} \tag{4.65}$$

We still let $U^n - u(t_n) = \theta^n + \rho^n$, where $\theta^n = U^n - \hat{u}(t_n)$ and $\rho^n = \hat{u}(t_n) - u(t_n)$. Then θ^n satisfies that $\theta^0 = 0$ and

$$i\varepsilon(\bar{\partial}\theta^n, w) + i\varepsilon(z_1^n, w) + i\varepsilon(z_3^n, w) = a\left(\frac{\theta^n + \theta^{n-1}}{2}, w\right), \quad \forall w \in \Psi_H, n = 1, \ldots, N, \tag{4.66}$$

where $z_1^n = \bar{\partial}\hat{u}(t_n) - \bar{\partial}u(t_n)$ and $z_3^n = \bar{\partial}u(t_n) - \frac{u_t(t_n)+u_t(t_{n-1})}{2}$.

For the L^2 error of U^N, we have the following theorem.

Theorem 4.5. Assume that U^N is the solution of (4.65) and u is the solution of (2.1). If $u_t(t), u_{tt}(t), u_{ttt}(t) \in L^2(\Omega)$ for any $t \in [0,T]$, then

$$||U^N - u(T)|| \leq C\left(\frac{\varepsilon\Delta t^2}{\min\{\varepsilon^4,\delta^4\}} + \frac{H^2}{\varepsilon\min\{\varepsilon^2,\delta^2\}}\right). \tag{4.67}$$

Moreover, If $u_t(t), u_{tt}(t) \in H^1(\Omega)$ for any $t \in [0,T]$, then

$$||U^N - u(T)|| \leq C\left(\frac{\varepsilon\Delta t^2}{\min\{\varepsilon^4,\delta^4\}} + \frac{H^3}{\varepsilon^2\delta\min\{\varepsilon^2,\delta^2\}}\right). \tag{4.68}$$

Proof. First consider the case where $u_t(t), u_{tt}(t), u_{ttt}(t) \in L^2(\Omega), \forall t \in [0,T]$. We have $||U^n - u(t_n)|| \leq ||\theta^n|| + ||\rho^n||$ and $||\rho^N|| \leq C\frac{H^2}{\varepsilon^2}$, $\theta^0 = 0$. Setting $w = \theta^n + \theta^{n-1}$ in (4.66) and taking the imaginary part of it, we have $\mathrm{Re}(\bar{\partial}\theta^n, \theta^n + \theta^{n-1}) = -\mathrm{Re}(z_1^n + z_3^n, \theta^n + \theta^{n-1})$, which implies

$$\frac{1}{\Delta t}(||\theta^n||^2 - ||\theta^{n-1}||^2) \leq (||\theta^n|| + ||\theta^{n-1}||)(||z_1^n|| + ||z_3^n||) \tag{4.69}$$

and hence

$$||\theta^N|| \leq ||\theta^0|| + \Delta t\sum_{n=1}^{N}(||z_1^n|| + ||z_3^n||). \tag{4.70}$$

By the proof of Theorem 4.3, we have $\Delta t\sum_{n=1}^N ||z_1^n|| \leq \frac{CH^2}{\varepsilon\min\{\varepsilon^2,\delta^2\}}$. For $||z_3^n||$, $n = 1, 2, \ldots, N$, we have

$$\begin{aligned}
||z_3^n|| &= \frac{1}{2\Delta t}||2(u(t_n) - u(t_{n-1})) - \Delta t(u_t(t_n) + u_t(t_{n-1}))|| \\
&\leq \frac{1}{2\Delta t}\Big(\int_{t_{n-\frac{1}{2}}}^{t_n}(t_n - s)^2||u_{ttt}(s)||ds + \int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(s - t_{n-1})^2||u_{ttt}(s)||ds \\
&\quad + \Delta t\int_{t_{n-\frac{1}{2}}}^{t_n}(t_n - s)||u_{ttt}(s)||ds + \Delta t\int_{t_{n-1}}^{t_{n-\frac{1}{2}}}(s - t_{n-1})||u_{ttt}(s)||ds\Big) \\
&\leq C\Delta t^2\max_{0\leq t\leq T}||u_{ttt}(t)|| \leq \frac{C\varepsilon\Delta t^2}{\min\{\varepsilon^4,\delta^4\}},
\end{aligned} \tag{4.71}$$

and hence $\Delta t\sum_{n=1}^N ||z_3^n|| \leq \frac{C\varepsilon\Delta t^2}{\min\{\varepsilon^4,\delta^4\}}$. Combining all the above inequalities, we obtain

$$||U^N - u(T)|| \leq C\left(\frac{\varepsilon\Delta t^2}{\min\{\varepsilon^4,\delta^4\}} + \frac{H^2}{\varepsilon\min\{\varepsilon^2,\delta^2\}}\right). \tag{4.72}$$

Moreover, if $u_t(t), u_{tt}(t) \in H^1(\Omega)$ for any $t \in [0,T]$, then from the proof of Theorem 4.3, we already know that $||\rho^N|| \leq C\frac{H^3}{\varepsilon^3\delta}$ and $\Delta t\sum_{n=1}^N ||z_1^n|| \leq \frac{CH^3}{\varepsilon^2\delta\min\{\varepsilon^2,\delta^2\}}$. Using similar arguments, we can prove the estimate in (4.68). □

For the error in the energy norm, we have the following theorem.

Theorem 4.6. Assume that U^N is the solution of (4.65) and u is the solution of (2.1). If $u_t(t), u_{tt}(t), u_{ttt}(t), u_{tttt}(t) \in L^2(\Omega)$ for any $t \in [0,T]$, then

$$||U^N - u(T)||_e \le C\left(\frac{H}{\varepsilon} + \frac{H^2}{\min\{\varepsilon^3, \delta^3\}} + \frac{\varepsilon^2 \Delta t^2}{\min\{\varepsilon^5, \delta^5\}}\right). \tag{4.73}$$

Moreover, if $u_t(t), u_{tt}(t), u_{ttt}(t) \in H^1(\Omega)$ for any $t \in [0,T]$, then

$$||U^N - u(T)||_e \le C\left(\frac{H^2}{\varepsilon^2 \delta} + \frac{H^3}{\varepsilon\delta \min\{\varepsilon^3, \delta^3\}} + \frac{\varepsilon^2 \Delta t^2}{\min\{\varepsilon^5, \delta^5\}}\right). \tag{4.74}$$

Proof. First consider the case where $u_t(t), u_{tt}(t), u_{ttt}(t), u_{tttt}(t) \in L^2(\Omega), \forall t \in [0,T]$. We have $||U^n - u(t_n)||_e \le ||\theta^n||_e + ||\rho^n||_e$, where $||\rho^N||_e \le C\frac{H}{\varepsilon}$. Setting $w = \theta^n - \theta^{n-1}$ in (4.66) and taking the real part of it, we have

$$||\theta^n||_e^2 \le ||\theta^{n-1}||_e^2 + 2\varepsilon|(z_1^n + z_3^n, \theta^n - \theta^{n-1})| \le ||\theta^{n-1}||_e^2 + 2\varepsilon||\theta^n - \theta^{n-1}||(||z_1^n|| + ||z_3^n||). \tag{4.75}$$

For $||\theta^n - \theta^{n-1}||$, we can derive by (4.66) that

$$i\varepsilon(\bar\partial\theta^n - \bar\partial\theta^{n-1}, w) + i\varepsilon(z_1^n - z_1^{n-1}, w) + i\varepsilon(z_3^n - z_3^{n-1}, w) = a\left(\frac{\theta^n - \theta^{n-2}}{2}, w\right), \quad \forall w \in \Psi_H. \tag{4.76}$$

Setting $w = \bar\partial\theta^n + \bar\partial\theta^{n-1} = \frac{\theta^n - \theta^{n-2}}{\Delta t}$ in the last equality and taking the imaginary part of it, we have

$$||\bar\partial\theta^n||^2 - ||\bar\partial\theta^{n-1}||^2 \le (||\bar\partial\theta^n|| + ||\bar\partial\theta^{n-1}||)(||z_1^n - z_1^{n-1}|| + ||z_3^n - z_3^{n-1}||) \tag{4.77}$$

and hence

$$||\theta^n - \theta^{n-1}|| \le ||\theta^1 - \theta^0|| + \Delta t\sum_{j=2}^{n}(||z_1^j - z_1^{j-1}|| + ||z_3^j - z_3^{j-1}||). \tag{4.78}$$

For $||\theta^1 - \theta^0||$, we have by the proof of Theorem 4.5 that

$$||\theta^1 - \theta^0|| = ||\theta^1|| \le \Delta t(||z_1^1|| + ||z_3^1||) \le C\left(\frac{\varepsilon\Delta t^3}{\min\{\varepsilon^4, \delta^4\}} + \frac{\Delta t H^2}{\varepsilon\min\{\varepsilon^2, \delta^2\}}\right), \tag{4.79}$$

and in the proof of Theorem 4.4 we know that $\Delta t\sum_{j=2}^n ||z_1^j - z_1^{j-1}|| \le \frac{C\Delta t H^2}{\min\{\varepsilon^4, \delta^4\}}$. For the term $\Delta t\sum_{j=2}^n ||z_3^j - z_3^{j-1}||$, we have that

$$\begin{aligned}
||z_3^j - z_3^{j-1}|| &= \frac{1}{2\Delta t}||2(u(t_j) - 2u(t_{j-1}) + u(t_{j-2})) - \Delta t(u_t(t_j) - u_t(t_{j-2}))|| \\
&\le \frac{1}{12\Delta t}\Big(2\int_{t_{j-1}}^{t_j}(t_j - s)^3||u_{tttt}(s)||ds + 2\int_{t_{j-2}}^{t_{j-1}}(s - t_{j-2})^3||u_{tttt}(s)||ds \\
&+ 3\Delta t\int_{t_{j-1}}^{t_j}(t_j - s)^2||u_{tttt}(s)||ds + 3\Delta t\int_{t_{j-2}}^{t_{j-1}}(s - t_{j-2})^2||u_{tttt}(s)||ds\Big) \\
&\le C\Delta t^3\max_{0\le t\le T}||u_{tttt}(t)|| \le C\frac{\varepsilon^2\Delta t^3}{\min\{\varepsilon^6, \delta^6\}}.
\end{aligned} \tag{4.80}$$

Therefore

$$||\theta^N||_e^2 \leq ||\theta^0||_e^2 + C\varepsilon \left(\frac{\Delta t H^2}{\min\{\varepsilon^4, \delta^4\}} + \frac{\varepsilon^2 \Delta t^3}{\min\{\varepsilon^6, \delta^6\}} \right) \sum_{n=1}^{N} (||z_1^n|| + ||z_3^n||). \tag{4.81}$$

By the proof of Theorem 4.5, we have $\Delta t \sum_{n=1}^{N} ||z_1^n|| \leq \frac{CH^2}{\varepsilon \min\{\varepsilon^2, \delta^2\}}$ and $\Delta t \sum_{n=1}^{N} ||z_3^n|| \leq \frac{C\varepsilon \Delta t^2}{\min\{\varepsilon^4, \delta^4\}}$. Therefore, we obtain

$$||U^N - u(T)||_e \leq C \left(\frac{H}{\varepsilon} + \frac{H^2}{\min\{\varepsilon^3, \delta^3\}} + \frac{\varepsilon^2 \Delta t^2}{\min\{\varepsilon^5, \delta^5\}} \right). \tag{4.82}$$

Moreover, if $u_t(t), u_{tt}(t), u_{ttt}(t) \in H^1(\Omega)$ for any $t \in [0, T]$, then from the proof of Theorem 4.4, we know that

$$||\rho^N||_e \leq C \frac{H^2}{\varepsilon^2 \delta}, \quad ||\theta^1 - \theta^0|| \leq C \left(\frac{\varepsilon \Delta t^3}{\min\{\varepsilon^4, \delta^4\}} + \frac{\Delta t H^3}{\varepsilon^2 \delta \min\{\varepsilon^2, \delta^2\}} \right), \tag{4.83}$$

$$\Delta t \sum_{j=2}^{n} ||z_1^j - z_1^{j-1}|| \leq \frac{C \Delta t H^3}{\varepsilon \delta \min\{\varepsilon^4, \delta^4\}}, \quad \Delta t \sum_{n=1}^{N} ||z_1^n|| \leq \frac{CH^3}{\varepsilon^2 \delta \min\{\varepsilon^2, \delta^2\}}. \tag{4.84}$$

Hence we can obtain (4.74) using similar arguments. □

Remark 4.1. For the estimates in Theorems 4.3, 4.4, 4.5 and 4.6, the constants C depend polynomially and at most quadratically on the final time T.

All the analyses in Sections 2, 3 and 4 can be performed with slight modifications for the Schrödinger equation (2.1) with zero boundary condition. The convergence results are the same as those in Section 4.

5. Numerical experiments

In this section, we present numerical results to justify our analysis, where the potential is smooth in one example and possesses discontinuities in the other. We consider (2.1) in one dimension with domain $\Omega = [0, 2\pi]$, finial time $T = 0.5$ and initial data

$$u_0(x) = \left(\frac{10}{\pi} \right)^{1/4} e^{-5(x-\pi)^2}. \tag{5.1}$$

And we shall compare the relative errors between the numerical solution ψ_{num} and the reference solution ψ_{ref} in L^2 norm and H^1 norm with

$$\text{err}_{L^2} = \frac{||\psi_{\text{num}} - \psi_{\text{ref}}||}{||\psi_{\text{ref}}||}, \quad \text{err}_{H^1} = \frac{||\psi_{\text{num}} - \psi_{\text{ref}}||_{H^1}}{||\psi_{\text{ref}}||_{H^1}}. \tag{5.2}$$

Recall that the H^1 norm is equivalent to the energy norm.

5.1. Smooth potentials

Consider the smooth potential

$$V = \cos\left(\frac{x}{\delta}\right) + 2. \tag{5.3}$$

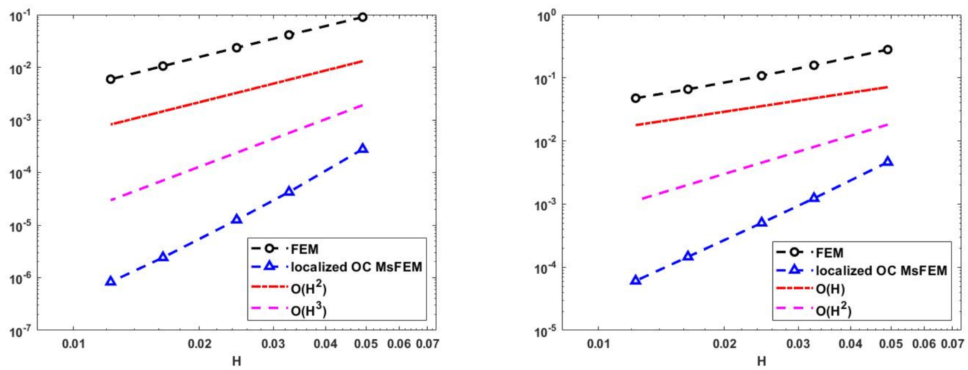
We choose (i) $\varepsilon = \frac{1}{8}, \delta = \frac{1}{10}$ and (ii) $\varepsilon = \frac{1}{32}, \delta = \frac{1}{24}$. The reference solution is computed by the time-splitting spectral method [1] with $\Delta t = \frac{1}{2^{26}}, H = \frac{\pi}{2^{15}}$. As for the numerical solution, Crank-Nicolson is adopted for temporal discretization with $\Delta t = \frac{1}{2^{24}}$ and for spatial discretization, the standard linear FEM and the localized OC MsFEM are used. The mesh size $H = \frac{\pi}{64}, \frac{\pi}{96}, \frac{\pi}{128}, \frac{\pi}{192}, \frac{\pi}{256}$ for case (i) and $H = \frac{\pi}{96}, \frac{\pi}{128}, \frac{\pi}{192}, \frac{\pi}{256}, \frac{\pi}{384}$ for case (ii). The oversampling size for the localized OC MsFEM is chosen as $m = 3\lceil \log_2(\frac{2\pi}{H})\rceil$. The results are shown in Tables 1, 2 and Figures 1, 2.

Table 1: Errors for potential (5.3) with $\varepsilon = 1/8, \delta = 1/10$

H	$\frac{\pi}{64}$	$\frac{\pi}{96}$	$\frac{\pi}{128}$	$\frac{\pi}{192}$	$\frac{\pi}{256}$
err_{L^2} of FEM	8.9746E-02	4.1331E-02	2.3531E-02	1.0562E-02	5.9291E-03
convergence order		1.91	1.96	1.84	2.25
err_{L^2} of localized OC MsFEM	2.7727E-04	4.2500E-05	1.2564E-05	2.4172E-06	8.3025E-07
convergence order		4.63	4.24	3.78	4.16
err_{H^1} of FEM	2.7996E-01	1.5785E-01	1.0777E-01	6.5908E-02	4.7552E-02
convergence order		1.41	1.33	1.13	1.27
err_{H^1} of localized OC MsFEM	4.6115E-03	1.2306E-03	5.0256E-04	1.4598E-04	6.0666E-05
convergence order		3.26	3.11	2.83	3.42

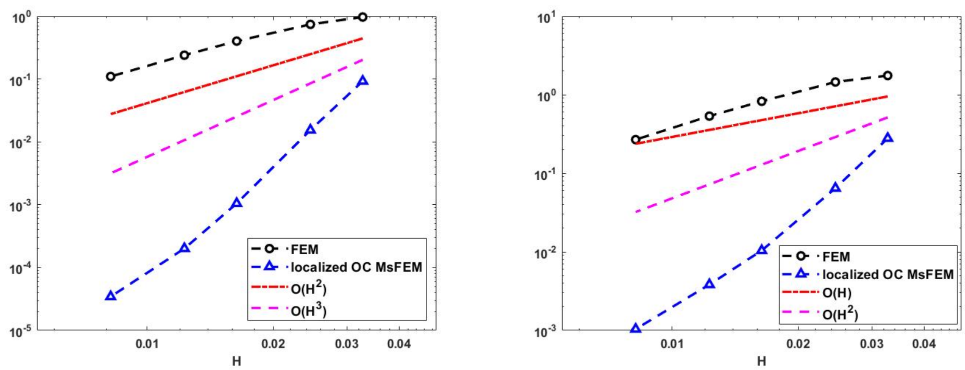
Table 2: Errors for potential (5.3) with $\varepsilon = 1/32, \delta = 1/24$

H	$\frac{\pi}{96}$	$\frac{\pi}{128}$	$\frac{\pi}{192}$	$\frac{\pi}{256}$	$\frac{\pi}{384}$
err_{L^2} of FEM	9.6768E-01	7.3988E-01	4.0070E-01	2.3916E-01	1.0963E-01
convergence order		0.93	1.41	2.01	1.79
err_{L^2} of localized OC MsFEM	9.2324E-02	1.5400E-02	1.0472E-03	2.0084E-04	3.4424E-05
convergence order		6.23	6.16	6.43	4.04
err_{H^1} of FEM	1.7538E+00	1.4517E+00	8.2473E-01	5.3417E-01	2.6809E-01
convergence order		0.66	1.30	1.69	1.58
err_{H^1} of localized OC MsFEM	2.7853E-01	6.4586E-02	1.0395E-02	3.8315E-03	1.0388E-03
convergence order		5.08	4.19	3.88	2.99



(a) L^2 relative error err_{L^2} (b) H^1 relative error err_{H^1}

Figure 1: Errors for potential (5.3) with $\varepsilon = 1/8, \delta = 1/10$



(a) L^2 relative error err_{L^2} (b) H^1 relative error err_{H^1}

Figure 2: Errors for potential (5.3) with $\varepsilon = 1/32, \delta = 1/24$

For the standard linear FEM, first-order convergence in the energy norm and second-order convergence in the L^2 norm are observed. While for the localized OC MsFEM, super convergence is observed and the convergence rates are even higher than the estimates (4.68), (4.74) proposed in Theorems 4.5 and 4.6. This super-convergence behavior is due to the smoothness of the potential (5.3) that results in a solution with high regularity. Sharper error estimates for solutions with sufficiently high regularity will be studied in our future work.

5.2. Discontinuous Potentials

Consider the potential

$$V = |x-\pi|^2 + 2 + \begin{cases} \cos\left(\dfrac{x}{\delta_1}\right), & x \in [0,\pi], \\ \cos\left(\dfrac{x}{\delta_2}\right), & x \in (\pi, 2\pi]. \end{cases} \tag{5.4}$$

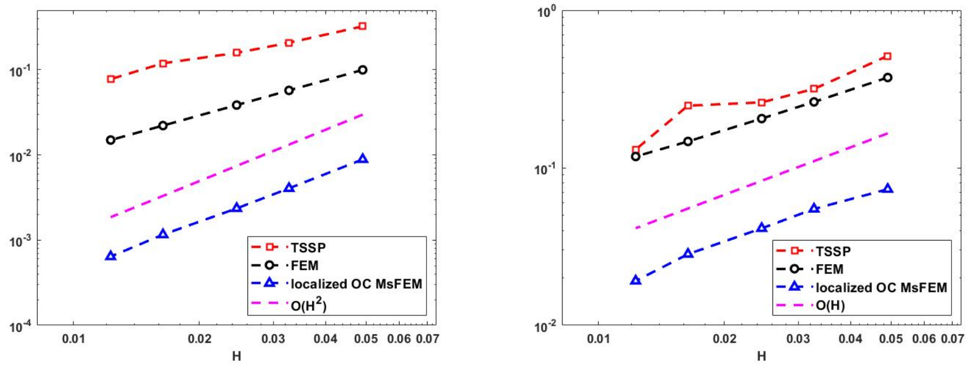
We choose (i) $\varepsilon = \frac{1}{8}, \delta_1 = \frac{1}{5}, \delta_2 = \frac{1}{10}$ and (ii) $\varepsilon = \frac{1}{32}, \delta_1 = \frac{1}{40}, \delta_2 = \frac{1}{25}$. In both cases, the potential (5.4) is discontinuous at $x = \pi$ and has different lattice structures on $[0, \pi]$ and $(\pi, 2\pi]$. The reference solution is computed by the Crank-Nicolson global OC MsFEM with $\Delta t = \frac{1}{2^{26}}, H = \frac{\pi}{1024}$. The numerical solutions are computed by the time-splitting spectral method (TSSP), Crank-Nicolson standard linear FEM and Crank-Nicolson localized OC MsFEM with $\Delta t = \frac{1}{2^{24}}$ and $H = \frac{\pi}{64}, \frac{\pi}{96}, \frac{\pi}{128}, \frac{\pi}{192}, \frac{\pi}{256}$ for case (i), $H = \frac{\pi}{96}, \frac{\pi}{128}, \frac{\pi}{192}, \frac{\pi}{256}, \frac{\pi}{384}$ for case (ii). The oversampling size for the localized OC MsFEM is chosen as $m = 3\lceil \log_2(\frac{2\pi}{H}) \rceil$. The results are shown in Tables 3, 4 and Figures 3, 4.

Table 3: Errors for potential (5.4) with $\varepsilon = 1/8, \delta_1 = 1/5, \delta_2 = 1/10$

H	$\frac{\pi}{64}$	$\frac{\pi}{96}$	$\frac{\pi}{128}$	$\frac{\pi}{192}$	$\frac{\pi}{256}$
err_{L^2} of TSSP	3.2300E-01	2.0757E-01	1.5783E-01	1.1911E-01	7.7628E-02
convergence order		1.09	0.95	0.65	1.67
err_{L^2} of FEM	9.9626E-02	5.7224E-02	3.8492E-02	2.2103E-02	1.4957E-02
convergence order		1.37	1.38	1.27	1.52
err_{L^2} of localized OC MsFEM	8.8678E-03	4.0528E-03	2.3565E-03	1.1604E-03	6.4039E-04
convergence order		1.93	1.88	1.62	2.31
err_{H^1} of TSSP	5.1257E-01	3.1662E-01	2.5999E-01	2.4780E-01	1.3052E-01
convergence order		1.19	0.68	0.11	2.50
err_{H^1} of FEM	3.7388E-01	2.6184E-01	2.0516E-01	1.4690E-01	1.1789E-01
convergence order		0.88	0.85	0.77	0.86
err_{H^1} of localized OC MsFEM	7.3066E-02	5.4768E-02	4.1242E-02	2.8283E-02	1.9120E-02
convergence order		0.71	0.99	0.86	1.52

Table 4: Errors for potential (5.4) with $\varepsilon = 1/32, \delta_1 = 1/40, \delta_2 = 1/25$

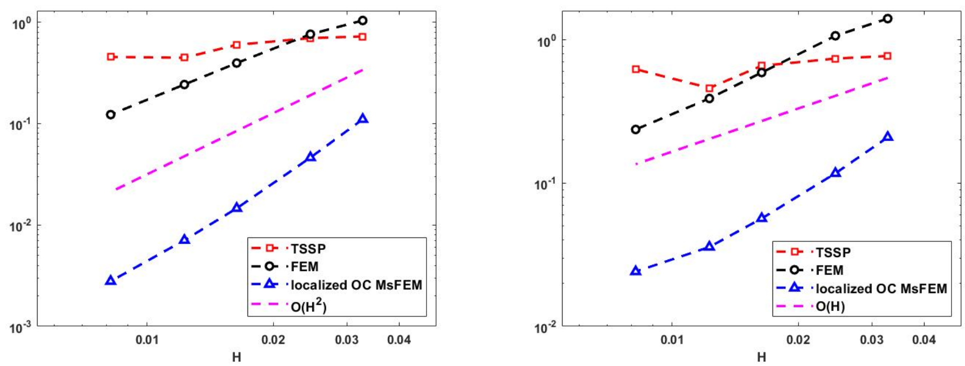
H	$\frac{\pi}{96}$	$\frac{\pi}{128}$	$\frac{\pi}{192}$	$\frac{\pi}{256}$	$\frac{\pi}{384}$
err_{L^2} of TSSP	7.2386E-01	6.9766E-01	5.9891E-01	4.4621E-01	4.5438E-01
convergence order		0.13	0.35	1.15	-0.04
err_{L^2} of FEM	1.0405E+00	7.6181E-01	3.9576E-01	2.4296E-01	1.2263E-01
convergence order		1.08	1.50	1.90	1.57
err_{L^2} of localized OC MsFEM	1.1020E-01	4.6191E-02	1.4599E-02	7.0645E-03	2.7841E-03
convergence order		3.02	2.64	2.83	2.13
err_{H^1} of TSSP	7.7187E-01	7.4138E-01	6.5957E-01	4.6178E-01	6.2428E-01
convergence order		0.14	0.27	1.39	-0.69
err_{H^1} of FEM	1.4094E+00	1.0687E+00	5.9197E-01	3.8997E-01	2.3699E-01
convergence order		0.96	1.35	1.62	1.14
err_{H^1} of localized OC MsFEM	2.0905E-01	1.1702E-01	5.6644E-02	3.5799E-02	2.4102E-02
convergence order		2.02	1.66	1.79	0.91



(a) L^2 relative error err_{L^2}

(b) H^1 relative error err_{H^1}

Figure 3: Errors for potential (5.4) with $\varepsilon = 1/8, \delta_1 = 1/5, \delta_2 = 1/10$



(a) L^2 relative error err_{L^2}

(b) H^1 relative error err_{H^1}

Figure 4: Errors for potential (5.4) with $\varepsilon = 1/32, \delta_1 = 1/40, \delta_2 = 1/25$

The time-splitting spectral method suffers from reduced convergence order and low accuracy due to the discontinuous potential (5.4). However, convergence rates of first order in the energy norm and second order in the L^2 norm are still observed for the FEM and OC MsFEM although the discontinuous potential (5.4) results in a solution with lower regularity. Moreover, the OC MsFEM yields much higher accuracy than the FEM, which is consistent with the analysis in Section 4.1.

Both examples confirm our theoretical findings and indicate that the OC MsFEM is accurate and robust for the Schrödinger equation with general multiscale potentials.

6. Conclusion

In this paper, we provide a rigorous convergence analysis for the OC MsFEM in solving Schrödinger equations with multiscale potentials in the semiclassical regime. We prove the exponential decay of the multiscale basis functions and propose the way of constructing the localized multiscale basis functions. Besides, we show that the localized basis functions can achieve the same accuracy as the global ones by choosing the oversampling size m appropriately according to the mesh size H as $m = O(\log(1/H))$. Based on the properties of Clément-type interpolation, we prove that the OC MsFEM can achieve first-order convergence in energy norm and second-order convergence in L^2 norm. Furthermore, if the solution possesses sufficiently high regularity, super convergence rates of second order in energy norm and third order in L^2 norm can be obtained. We find that using the same mesh size the OC MsFEM gives more accurate results than the FEM in solving Schrödinger equations with multiscale potentials due to its super convergence behavior and weaker denendence on the small parameters ε and δ. Numerical results confirm our analysis. For a smooth potential, super convergence rates are observed for the OC MsFEM. While for a discontinuous potential, the OC MsFEM retains first-order and second-order convergence in the energy norm and L^2 norm respectively and still yields high accuracy. Therefore, the OC MsFEM is accurate and robust for the Schrödinger equation with various types of multiscale potentials.

In the future, we will study the convergence analysis of the OC MsFEM for solving eigenvalue problems for the Schrödinger operators and nonlinear Schrödinger equations. In addition, we will apply the OC MsFEM to solve wave equations with multiscale features, such as the Klein-Gordon equation [21].

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