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 general multiscale potentials in the semiclassical regime. In the OC MsFEM the multiscale basis functions are reconstructed 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, which achieve the same accuracy as the global ones if the oversampling size $m = O(\log(1/H))$. We prove the first-order convergence in the energy norm and second-order convergence in the $L^2$ norm for the OC MsFEM and super convergence rates can be obtained if the solution possesses sufficiently high regularity. By analysing the regularity of the solution, we also derive the dependence of the error estimates on the small parameters of the Schrödinger equation. We find that the OC MsFEM outperforms the finite element method (FEM) due to the super convergence behavior for high-regularity solutions and weaker dependence on the small parameters for low-regularity solutions in the presence of the multiscale potential. Finally, we present numerical results to demonstrate the accuracy and robustness of the OC MsFEM.

Key words. Schrödinger equation; semiclassical regime; 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. A widely studied model is the electron motion in a perfect crystal with an external field, where the potential is a linear combination of an oscillatory periodic potential and a slowly-varying external potential. 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.
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 magnetoresistance [44], the silicon-based heterojunction for solar cells [27], and quantum metamaterials [39]. For the electron motion in these heterostructures, however, the potential 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.

In this paper, we consider the semiclassical Schrödinger equation with a general multiscale potential

\[
\begin{align*}
\mathcal{L}_\varepsilon u_{\varepsilon,\delta} &= -\frac{1}{2}\varepsilon^2 \nabla^2 u_{\varepsilon,\delta} + V^{\delta}(x)u_{\varepsilon,\delta}, \\
u_{\varepsilon,\delta}|_{t=0} &= u_{0,\varepsilon}(x), \quad x \in \mathbb{R}^d,
\end{align*}
\]

where \(0 < \varepsilon \ll 1\) is an effective Planck constant describing the microscopic/macrosopic scale ratio, \(u_{0,\varepsilon}(x)\) is the initial data that is dependent on the effective Planck constant \(\varepsilon\) (motivated by the WKB approximation), \(d\) is the spatial dimension, and \(V^{\delta}(x) \in \mathbb{R}\) is a general multiscale potential depending on the small parameter \(0 < \delta \ll 1\), which describes the multiscale structure in the potential and can be different from \(\varepsilon\). By assuming the dependence of the potential on \(\delta\), we can see in the subsequent analysis how the multiscale potential \(V^{\delta}\) influences the regularity of the solution and hence the error estimates of different numerical methods.

For the numerical solution of (1.1), traditional methods like the FEM [9] and finite difference method (FDM) [29, 30] are prohibitively costly due to the strong mesh size restrictions induced by the small effective Planck constant and multiscale structures 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 \(V^{\delta}(x)\) in a general form, an 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 \(\mathcal{H} = -\frac{1}{2}\varepsilon^2 \Delta + V^{\delta}(x)\). The fully discrete scheme can be given with a finite difference scheme in temporal discretization, e.g. the 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 for arbitrary bounded multiscale potentials
and thus the OC MsFEM for the Schrödinger equation can be applied to a multiscale potential \( V^\delta \) 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 approx-
imation error of the OC MsFEM for the semiclassical Schrödinger equation with multiscale
potentials.

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 estimates on the small
parameters \( \varepsilon \) and \( \delta \). 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 for high-regularity solutions and weaker dependence on the
small parameters \( \varepsilon \) and \( \delta \) for low-regularity solutions. The weaker dependence of the OC
MsFEM on the small parameters results from the fact that the projection error estimate of
OC MsFEM depends on higher temporal regularity of the solution while the projection error
estimate of FEM depends on higher spatial regularity of solution, and the fact that the spatial
derivatives of the solution are more oscillatory than the time derivatives in the presence of
the multiscale potential; see Lemmas 2.3, 2.4, 2.5, Remark 2.2 and the discussion in Section
4.1. Finally, we present numerical results to confirm our theoretical findings. The numerical
examples also show that the OC MsFEM is robust in the sense that it still yields high accuracy
for discontinuous multiscale potentials.

The rest of the paper is organized as follows. In Section 2, we will introduce the setting of
the problem and some preliminaries on the Clément-type interpolation, and we will also prove
some estimates of the regularity of the solution. In Section 3, we will prove the exponential
deay of the global basis functions and discuss the approximation property of the projection
in both global and localized multiscale space. Then, we will study the convergence rates of
the OC MsFEM for the Schrödinger equation in Section 4. 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 preparations

In this section, the problem setting of the semiclassical Schrödinger equation with a mul-
tiscale potential is formulated. Then some results on the Clément-type interpolation are
introduced. In addition, we prove some estimates of the regularity of the solution.
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 $D_x^\sigma$, where $D_x^\sigma w = \partial_{x_1}^{\sigma_1} \cdots \partial_{x_d}^{\sigma_d} w$ with the multi-index $\sigma = (\sigma_1, \ldots, \sigma_d) \in \mathbb{N}^d$ and $|\sigma| = \sigma_1 + \cdots + \sigma_d$. 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 $L^\infty$ norm with $||w||_\infty = \text{ess sup}_{x \in \Omega} |w(x)|$ and the spatial $H^k$ norm is denoted by $|| \cdot ||_{H^k}$ with $||w||^2_{H^k} = ||w||^2 + \sum_{0 \leq |\sigma| \leq k} ||D_x^\sigma w||^2$. 

For any $u \in H^1(\Omega)$, the energy norm with $(\cdot, \cdot)$ is denoted by $||w||_e = ||w||_1$.

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:

$$
\begin{cases}
  i\varepsilon \partial_t u^{\varepsilon, \delta} = -\frac{1}{2} \varepsilon^2 \Delta u^{\varepsilon, \delta} + V^\delta(x) u^{\varepsilon, \delta}, & x \in \Omega, 0 < t \leq T, \\
  u^{\varepsilon, \delta}, D_x^\sigma u^{\varepsilon, \delta} \text{ are periodic on } \partial \Omega, & |\sigma| = 1, 0 < t \leq T, \\
  u^{\varepsilon, \delta}|_{t=0} = u_0^{\varepsilon}(x), x \in \Omega.
\end{cases}
$$

We assume that $u_0^{\varepsilon}(x)$ satisfies $||D_x^\sigma u_0^{\varepsilon}|| \leq \frac{C}{\varepsilon |\sigma|}$. And for the multiscale potential $V^\delta$, we assume that $V_{\min} \leq V^\delta(x) \leq V_{\max}$, $\forall x \in \Omega$, where $0 < V_{\min} \leq V_{\max}$ and $||D_x^\sigma V^\delta||_\infty \leq \frac{C}{\delta |\sigma|}$. Moreover, we assume that $D_x^\sigma u^{\varepsilon, \delta}$ are periodic on $\partial \Omega$ for $|\sigma| = 2, 3$ and $0 < t \leq T$.

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

In the following, for brevity of notations, the superscripts $\varepsilon, \delta$ will be dropped for $u_0^{\varepsilon}, u^{\varepsilon, \delta}$ and $V^\delta$ unless necessary. We introduce the bilinear form associated with the Schrödinger operator $\mathcal{H} = -\frac{1}{2} \varepsilon^2 \Delta + V$ as

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

The following energy norm is introduced:

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

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 $v, w \in H^1(\Omega)$,

$$|a(v, w)| \leq ||v||_e ||w||_e. \quad (2.4)$$
If the stationary problem with $\mathcal{H}$ as the differential operator
\begin{equation}
\begin{aligned}
\mathcal{H}u &= f, \quad x \in \Omega, \\
u, D_x^\sigma u \text{ are periodic on } \partial \Omega, |\sigma| = 1,
\end{aligned}
\end{equation}
is considered, where periodic boundary conditions are prescribed and $f \in L^2(\Omega)$, the associated variational problem would be to find $u \in H^1_p(\Omega)$ such that
\begin{equation}
a(u, v) = (f, v), \quad \forall v \in H^1_p(\Omega).
\end{equation}
By the Lax-Milgram theorem, the variational problem (2.6) admits a unique solution $u \in H^1_p(\Omega)$ with a stability estimate
\begin{equation}
||u||_e \leq C_{\text{st}}(\varepsilon, V)||f||.
\end{equation}

2.2. Clément-type interpolation

Let $T_H = \{T_e\}_{e=1}^{N_e}$ be some quasi-uniform and shape-regular simplicial finite element meshes [6, 13, 14] of $\Omega$ with mesh size $H$, where $N_e$ is the number of elements. Then for $K$ being the union of some elements in $T_H$, the neighbourhood of $K$ can be defined as
\begin{equation}
N(K) = \bigcup_{G \in T_H, G \cap K \neq \emptyset} G.
\end{equation}
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
\begin{equation}
\eta(x) = \frac{\text{dist}(x, N^m(K))}{\text{dist}(x, N^m(K)) + \text{dist}(x, \Omega \setminus N^{m+1}(K))}
\end{equation}
for some $m \in \mathbb{N}$, the shape regularity of $T_H$ implies that $H||\nabla \eta||_{\infty} \leq \gamma$, where $\gamma$ is independent of $\varepsilon, \delta, m$ and $H$. The shape regularity and quasi-uniformness also imply that there exists a constant $C_{\text{ol}}$ independent of $\varepsilon, \delta, m$ and $H$ [36, 37] such that
\begin{equation}
\max_{T \in T_H} \text{card}\{G \in T_H | G \subset N(T)\} \leq C_{\text{ol}}.
\end{equation}

The first-order conforming finite element space of $T_H$ is given by
\begin{equation}
\Phi_H = \{\phi \in H^1_p(\Omega) | \forall T \in T_H, \phi|_T \text{ is a polynomial of total degree } \leq 1\}.
\end{equation}
Let $N_H$ be the set of vertices of $T_H$ with repeated vertices due to the periodic boundary conditions removed and $N_H = |N_H|$. Then $\Phi_H = \text{span}\{\phi_j, j = 1, \ldots, N_H\}$, where $\phi_j \in \Phi_H, j = 1, \ldots, N_H$ is the nodal basis satisfying $\phi_j(x_k) = \delta_{jk}, \forall x_k \in N_H$. The Clément-type interpolation operator $I_H$ [2, 7, 40] is defined by
\begin{equation}
I_H v = \sum_{j=1}^{N_H} \alpha_j(v) \phi_j, \quad \forall v \in H^1_p(\Omega),
\end{equation}
where \( \alpha_j(v) = \frac{(v, \phi_j)}{(\overline{v}, \phi_j)} \). Then, the local approximation and stability properties of the interpolation operator \( I_H [3] \) guarantee that there exists a constant \( C_I \) only depending on the shape regularity such that
\[
H^{-1}||v - I_H v||_T + ||\nabla(v - I_H v)||_T \leq C_I ||\nabla v||_{N(T)}, \quad \forall T \in \mathcal{T}_H, \tag{2.13}
\]
where \( (v, w)_K = \int_K v \overline{w} \) 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 \( \mathcal{W} = \ker(I_H) \). Then \( H^1 P(\Omega) = \Phi \oplus \mathcal{W} \) and \( (v, w) = 0, \forall v \in \Phi, w \in \mathcal{W} \). We have the following lemma.

**Lemma 2.2.** For \( v \in \mathcal{W}, f \in L^2(\Omega) \), there holds
\[
(f, v) \leq C_H ||f|| ||\nabla v||. \tag{2.14}
\]
Moreover, if \( f \in H^1(\Omega) \), then
\[
(f, v) \leq C_H^2 ||\nabla f|| ||\nabla v||. \tag{2.15}
\]

**Proof.** Since \( v \in \mathcal{W} \), then \( I_H v = 0 \). By (2.10) and (2.13), we have
\[
(f, v) = (f, v - I_H v) \leq ||f|| ||v - I_H v|| \leq C_H ||f|| ||\nabla v||. \tag{2.16}
\]
Note that \( (I_H f, v) = 0 \). Hence if we further have \( f \in H^1(\Omega) \), then
\[
(f, v) = (f - I_H f, v - I_H v) \leq C_H^2 ||\nabla f|| ||\nabla v||. \tag{2.17}
\]

Moreover, there exists a local right inverse of \( I_H [16] \), denoted by \( I_{H, loc}^{-1} : \Phi \to H^1 P(\Omega) \), satisfying
\[
I_H(I_{H, loc}^{-1} v_H) = v_H, \tag{2.18}
\]
\[
||\nabla I_{H, loc}^{-1} v_H|| \leq C'_{I_H} ||\nabla v_H||, \tag{2.19}
\]
\[
supp(I_{H, loc}^{-1} v_H) = \bigcup\{T \in \mathcal{T}_H | T \cap \overline{supp(v_H)} \neq \emptyset\}, \tag{2.20}
\]
where \( v_H \in \Phi \) and \( C'_{I_H} \) only depends on the shape regularity.

### 2.3. Regularity of the solutions of Schrödinger equations with multiscale potentials

We are interested in studying the dependence of the error estimates of OC MsFEM on the small parameters \( \varepsilon, \delta \). Hence we need to study the temporal and spatial regularity of the solution \( u \) of the Schrödinger equation (2.1). We first study the temporal regularity of \( u \).

**Lemma 2.3.** 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 that for any \( 0 \leq t \leq T \)
\[
||\partial_t^k u(t)|| \leq \frac{C \varepsilon^{k-2}}{\min\{\varepsilon^{2k-2}, \delta^{2k-2}\}}, \tag{2.21}
\]
Proof. For \( u_t \), taking the time derivative of (2.1), multiplying it with \( \bar{u}_t \), integrating it w.r.t. \( x \) over \( \Omega \) and taking the imaginary part, we have

\[
\frac{d}{dt}||u_t||^2 = 0,
\]

which implies

\[
||u_t(t)|| = ||u_t(0)||, \quad \forall t \in [0,T].
\]

For \( ||u_t(0)|| \), we have

\[
i\varepsilon u_t(0) = -\frac{\varepsilon}{2} \Delta u_0 + Vu_0,
\]

which indicates

\[
||u_t(0)|| \leq \varepsilon \left( \frac{\varepsilon}{2} ||\Delta u_0|| + \frac{1}{\varepsilon} ||Vu_0|| \right) \leq \frac{C}{\varepsilon}. \tag{2.22}
\]

Applying similar procedures to \( u_{tt}, u_{ttt} \) and \( u_{tttt} \), we can obtain the results (2.21).

Then, we turn to the spatial regularity of \( u \).

**Lemma 2.4.** If \( D^\sigma_x u(t) \in L^2(\Omega) \) for any \( t \in [0,T] \) and \( |\sigma| = k \), where \( k = 1, 2 \), then it holds true that for any \( 0 \leq t \leq T \)

\[
||D^\sigma_x u(t)|| \leq \frac{C}{\varepsilon^k \delta^k}. \tag{2.23}
\]

**Proof.** For \( |\sigma| = 1 \), it is sufficient to prove (2.23) 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. \( x \) over \( \Omega \) and taking the imaginary part, we have

\[
\varepsilon \frac{1}{2} \frac{d}{dt} ||u_{x_1}||^2 = \text{Im}(V_{x_1} u, u_{x_1}). \tag{2.24}
\]

Then

\[
\frac{1}{2} \frac{d}{dt} ||u_{x_1}||^2 \leq \frac{1}{\varepsilon} |(V_{x_1} u, u_{x_1})| \leq \frac{1}{\varepsilon \delta} ||u|| ||u_{x_1}||,
\]

and hence

\[
\frac{d}{dt} ||u_{x_1}|| \leq \frac{1}{\varepsilon \delta} ||u||.
\]

Therefore, we have

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

which implies (2.23) for \( |\sigma| = 1 \). Then, applying the same procedure to any \( D^\sigma_x u \) with \( |\sigma| = 2 \), we obtain the result. \( \square \)

Furthermore, we have

**Lemma 2.5.** 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 that for any \( 0 \leq t \leq T \)

\[
||\nabla \partial^k_t u(t)|| \leq \frac{C \varepsilon^{k-2}}{\varepsilon \delta \min\{\varepsilon^{2k-2}, \delta^{2k-2}\}}. \tag{2.27}
\]

**Proof.** By combining the proofs of Lemma 2.3 and Lemma 2.4, we can obtain the result. \( \square \)

**Remark 2.2.** We can see from Lemmas 2.3, 2.4 and 2.5 that with the emergence of the multiscale potential, i.e. \( 0 < \delta \ll 1 \), the spatial derivatives of the solution become more oscillatory than the time derivatives.
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 \(H/\varepsilon \leq (2C_{l_H} \sqrt{C_{d_l} V_{\text{max}} (1 + C_{l_H} C_{d_l} \gamma)})^{-1}\).

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

**Lemma 3.1.** Under Assumption 3.1, for any \(v \in W\), we have
\[
\varepsilon ||\nabla v|| \leq ||v||_e \leq C\varepsilon ||\nabla v||.
\]

**Proof.** For any \(v \in W\), it is easy to see that \(\varepsilon ||\nabla v|| \leq ||v||_e\). On the other hand, by Lemma 2.2,
\[
||v||_e^2 \leq \frac{\varepsilon^2}{2} ||\nabla v||^2 + V_{\text{max}}(v,v) \leq C \left(1 + \frac{H^2}{\varepsilon^2} \right) \varepsilon^2 ||\nabla v||^2 \leq C\varepsilon^2 ||\nabla v||^2,
\]
which completes the proof.

### 3.1. Global multiscale finite element basis functions

For \(j = 1, \ldots, N_H\), the operator-compressed multiscale basis function \(\psi_j\) is constructed as the solution of the constrained optimization problem
\[
\min_{\psi \in H^1_p(\Omega)} a(\psi, \psi), \quad \text{s.t. } (\psi, \phi_k) = \delta_{jk}, \quad k = 1, \ldots, N_H.
\]

Define \(\Psi_H = \text{span}\{\psi_j, j = 1, \ldots, N_H\}\) as the global multiscale finite element space. We have the following lemma.

**Lemma 3.2.** \(H^1_p(\Omega) = \Psi_H \oplus W\) and for any \(v_H \in \Psi_H\) and \(w \in W\),
\[
a(v_H, w) = 0.
\]

**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
\[
g(\eta) = a(\psi_j + \eta w, \psi_j + \eta w) = \eta^2 a(w, w) + 2\eta \text{Re} a(\psi_j, w) + a(\psi_j, \psi_j).
\]

Since \(g(\eta)\) achieves the minimum at \(\eta = 0\), then \(g'(\eta)|_{\eta=0} = 0\). Hence \(\text{Re} a(\psi_j, w) = 0\). Set \(\tilde{\eta} = i\eta\) and \(\tilde{g}(\eta) = g(\tilde{\eta})\). A similar argument for \(\tilde{g}(\eta)\) yields that \(\text{Im} a(\psi_j, w) = 0\). Therefore, we have \(a(\psi_j, w) = 0, \quad j = 1, \ldots, N_H\), i.e.,
\[
a(v_H, w) = 0, \quad \forall v_H \in \Psi_H, w \in W.
\]

For any \(v \in H^1_p(\Omega)\), define \(v^* = \sum_{k=1}^{N_H} (v, \phi_k) \phi_k\). Then \(v^* \in \Psi_H\) and
\[
(v - v^*, \phi_j) = 0, \quad j = 1, \ldots, N_H.
\]

Then \(v - v^* \in W\) and hence we have the decomposition \(H^1_p(\Omega) = \Psi_H \oplus W\). 

\[\square\]
To solve the stationary problem \((2.5)\) in \(\Psi_H\), the Galerkin method seeks \(u_H \in \Psi_H\) such that
\[
a(u_H, v_H) = (f, v_H), \quad \forall v_H \in \Psi_H.
\] (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 \(\Psi_H\). Then \(u - u_H \in W\).

**Proof.** By Lemma 3.2, \(u - u_H \in W\) since
\[
a(u - u_H, w_H) = 0, \quad \forall w_H \in \Psi_H.
\]
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 2.2 we obtain
\[
||u - u_H||_e^2 = a(u - u_H, u - u_H) = a(u, u - u_H)
= (f, u - u_H) \leq CH||f||||\nabla(u - u_H)|| \leq C \frac{H}{\varepsilon} ||f|| ||u - u_H||_e. \tag{3.13}
\]
For the \(L^2\) error, the Aubin-Nitsche technique is applied. Let \(w \in H^1_P(\Omega)\) be the solution of
\[
a(w, v) = (u - u_H, v), \quad \forall v \in H^1_P(\Omega) \tag{3.14}
\]
and \(w_H \in \Psi_H\) be the Galerkin approximation of \(w\) in \(\Psi_H\) satisfying
\[
a(w_H, v_H) = (u - u_H, v_H), \quad \forall v_H \in \Psi_H. \tag{3.15}
\]
Then, we easily obtain
\[
||u - u_H||^2 = a(w, u - u_H) = a(w - w_H, u - u_H)
\leq ||w - w_H||_e ||u - u_H||_e \leq C \frac{H^2}{\varepsilon^2} ||f|| ||u - u_H||, \tag{3.16}
\]
where in the last equality we have used the estimate \((3.9)\). Moreover, if \(f \in H^1(\Omega)\), we have by Lemma 2.2 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 can obtain the results \((3.11)\) and \((3.12)\). \qed
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 $S_j = \text{supp}(\phi_j)$, where $\phi_j$ is the finite element nodal basis. We have the following theorem indicating the exponential decay of basis functions $\psi_j$.

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

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

**Proof.** The proof is based on an iterative Caccioppoli-type argument [18, 34, 36]. In this proof, we fix the index $j$ and omit $j$ for $\psi_j$ and $S_j$ for brevity of notations. Assume $m \geq 7$. Define the cutoff function

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

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

$$||\nabla \psi||_{\Omega \setminus N^m(S)} \leq (\nabla \psi, \eta \nabla \psi) = (\nabla \psi, \nabla (\eta \psi)) - (\nabla \psi, \psi \nabla \eta) \leq |(\nabla \psi, \nabla (\eta \psi - I^{-1}_{H, \text{loc}}(I_H(\eta \psi))))| + |(\nabla \psi, \nabla I^{-1}_{H, \text{loc}}(I_H(\eta \psi)))| + |(\nabla \psi, \psi \nabla \eta)| = M_1 + M_2 + M_3, \quad (3.20)$$

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

$$M_1 \leq \frac{2V_{\max}}{\varepsilon^2} |(\psi, w)| = \frac{2V_{\max}}{\varepsilon^2} |(\psi - I_H \psi, \eta \psi - I_H(\eta \psi) + I_H(\eta \psi) - I^{-1}_{H, \text{loc}}(I_H(\eta \psi)))| \leq \frac{2V_{\max}}{\varepsilon^2} \left( |(\psi - I_H \psi, \eta \psi - I_H(\eta \psi))| + |(\psi - I_H \psi, I_H(\eta \psi) - I^{-1}_{H, \text{loc}}(I_H(\eta \psi)))| \right) \leq 2V_{\max} C_{\text{rel}}^2 \frac{H^2}{\varepsilon^2} ||\nabla \psi||_{\Omega \setminus N^{m-6}(S)} ||\nabla (\eta \psi)||_{\Omega \setminus N^{m-6}(S)} + 2V_{\max} C_{\text{rel}}^3 \frac{H^2}{\varepsilon^2} ||\nabla \psi||_{N^{m}(S) \setminus N^{m-7}(S)} ||\nabla (\eta \psi)||_{N^{m}(S) \setminus N^{m-7}(S)}. \quad (3.21)$$
Also note that \( R \cap \text{supp}(I_H \psi) = \emptyset \) and hence
\[
|| \psi \nabla \eta ||_R = || (\psi - I_H \psi) \nabla \eta ||_R \leq C_{I_H} C_{\text{col}} \| \nabla \eta \|_\infty \| \nabla \psi \|_{N(R)} \leq C_{I_H} C_{\text{col}} \gamma \| \nabla \psi \|_{N(R)}. \tag{3.22}
\]

Thus, under Assumption 3.1, we arrive at
\[
M_1 \leq \frac{1}{2} \| \nabla \psi \|^2_{\Omega \setminus N^m(S)} + C \| \nabla \psi \|^2_{N^m(S) \setminus N^{m-\gamma}(S)}. \tag{3.23}
\]

Using a similar argument, we have
\[
M_2 \leq C \| \nabla \psi \|_{N^{m-1}(S) \setminus N^{m-6}(S)} \| \nabla (\eta \psi) \|_{N^{m-1}(S) \setminus N^{m-6}(S)} \leq C \| \nabla \psi \|^2_{N^m(S) \setminus N^{m-\gamma}(S)}, \tag{3.24}
\]
\[
M_3 \leq C \| \nabla \psi \|^2_{N^m(S) \setminus N^{m-\gamma}(S)}. \tag{3.25}
\]

Combining the above estimates, we get that
\[
\frac{1}{2} \| \nabla \psi \|^2_{\Omega \setminus N^m(S)} \leq C_1 \| \nabla \psi \|^2_{N^m(S) \setminus N^{m-\gamma}(S)}, \tag{3.26}
\]
where \( C_1 \) is independent of \( \varepsilon, \delta, m \) and \( H \). This leads to
\[
\| \nabla \psi \|_{\Omega \setminus N^m(S)}^2 \leq \frac{C_1}{C_1 + \frac{1}{2}} \| \nabla \psi \|_{\Omega \setminus N^{m-\gamma}(S)}^2, \tag{3.27}
\]
which implies
\[
\| \nabla \psi \|_{\Omega \setminus N^m(S)}^2 \leq \left( \frac{C_1}{C_1 + \frac{1}{2}} \right)^{\left[ \frac{m}{\gamma} \right]} \| \nabla \psi \|^2. \tag{3.28}
\]

Therefore, we prove that the basis functions \( \psi_j \)'s have the exponential decay property. \( \Box \)

3.2.2. Localized basis functions

Motivated by the exponential decay of the multiscale basis functions, we can construct the localized basis function \( \psi_{j, m}^{\text{loc}} \) by solving the modified constrained optimization problem
\[
\min_{\psi \in H^1_0(\Omega)} a(\psi, \psi), \tag{3.29}
\]
\[
\text{s.t. } (\psi, \phi_k) = \delta_{jk}, \quad k = 1, \ldots, N_H, \quad \psi(x) = 0, \quad \text{for } x \in \Omega \setminus N^m(S_j)
\]
for \( j = 1, \ldots, N_H \) and \( m \in \mathbb{N} \). Let \( W(N^m(S_j)) = \{ w \in W | w = 0 \text{ in } \Omega \setminus N^m(S_j) \} \).

For the proof of Lemma 3.2, we can prove the following lemma.

**Lemma 3.4.** It holds true that for \( j = 1, \ldots, N_H \)
\[
a(\psi_{j, m}^{\text{loc}}, w) = 0, \quad \forall w \in W(N^m(S_j)). \tag{3.30}
\]

Define \( \Psi_{H,m} = \text{span}\{ \psi_{j, m}^{\text{loc}}, j = 1, \ldots, N_H \} \) 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 \( j = 1, \ldots, N_H \)
\[
||\nabla \psi_j|| \leq CH^{-\frac{2}{d}}. \tag{3.31}
\]

Proof. Define the operator \( P \) as for any \( v \in H^1_p(\Omega) \), \( Pv \in W \) 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 \( P\hat{\psi}_j = 0, j = 1, \ldots, N_H \). We know that \( \{\hat{\psi}_j\}_{j=1}^{N_H} \) spans \( \Psi_H \) since \( \psi_j \)'s are linearly independent. Therefore
\[
\hat{\psi}_j = \sum_{k=1}^{N_H} \alpha_k^{(j)}(P\phi_k - \phi_k). \tag{3.33}
\]
Note that \( (\hat{\psi}_j, \phi_k) = \delta_{j,k} \). Then \( \sum_{k=1}^{N_H} (P\phi_k, \phi_k) = -\delta_{j,k} \). So if we let \( \alpha_k^{(j)} = (\alpha_1^{(j)}, \ldots, \alpha_k^{(j)}, \ldots, \alpha_{N_H}^{(j)}) \), then \( M\alpha_k^{(j)} = -e_j \), 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], we know that \( ||(M^{-1})_{j,k}|| \leq CH^{-d} \). Therefore, under Assumption 3.1, we have
\[
||\nabla \hat{\psi}_j|| \leq \sum_{k=1}^{N_H} \alpha_k^{(j)} ||\nabla (P\phi_k - \phi_k)|| \leq CN_H H^{-\frac{2}{d}} \leq CH^{-\frac{2}{d}}. \tag{3.34}
\]
\[
\square
\]
We also need two lemmas on the difference between \( \psi_j \) and \( \psi_j^{loc,m} \).

Lemma 3.6. Under Assumption 3.1, for \( j = 1, \ldots, N_H \), we have
\[
||\nabla (\psi_j - \psi_j^{loc,m})|| \leq CH^{-\frac{3}{2}d} \beta^m. \tag{3.35}
\]

Proof. Let \( m \geq 6 \) and \( \tilde{\psi}_j = \psi_j - I_H^{-1,loc}(I_H\psi_j) \) and \( \tilde{\psi}_j^{loc,m} = \psi_j^{loc,m} - I_H^{-1,loc}(I_H\tilde{\psi}_j^{loc,m}) \). Then \( \psi_j - \psi_j^{loc,m} = \tilde{\psi}_j - \tilde{\psi}_j^{loc,m} \) since \( I_H\psi_j = I_H\psi_j^{loc,m} = \phi_j/(1, \phi_j) \). In addition, \( \psi_j \in W \) and \( \tilde{\psi}_j^{loc,m} \in W(N^m(S_j)) \). Then \( \forall w \in W(N^m(S_j)) \),
\[
\varepsilon^2 ||\nabla (\tilde{\psi}_j - \tilde{\psi}_j^{loc,m})||^2 \leq a(\tilde{\psi}_j - \tilde{\psi}_j^{loc,m}, \tilde{\psi}_j - \tilde{\psi}_j^{loc,m}) = a(\tilde{\psi}_j - \tilde{\psi}_j^{loc,m}, \tilde{\psi}_j - w) \leq ||\tilde{\psi}_j - \tilde{\psi}_j^{loc,m}||_e ||\tilde{\psi}_j - w||_e \leq C\varepsilon^2 ||\nabla (\tilde{\psi}_j - \tilde{\psi}_j^{loc,m})|| ||\nabla (\tilde{\psi}_j - w)||, \tag{3.36}
\]
where we have used the fact that \( a(\psi_j, w - \tilde{\psi}_j^{loc,m}) = a(\psi_j^{loc,m}, w - \tilde{\psi}_j^{loc,m}) = 0 \) and hence \( a(\tilde{\psi}_j - \psi_j^{loc,m}, w - \tilde{\psi}_j^{loc,m}) = a(\psi_j - \psi_j^{loc,m}, w - \tilde{\psi}_j^{loc,m}) = 0 \).

Define the cutoff function
\[
\eta = \frac{\text{dist}(x, \Omega \setminus N^{m-2}(S_j))}{\text{dist}(x, N^{m-3}(S_j)) + \text{dist}(x, \Omega \setminus N^{m-2}(S_j))}. \tag{3.37}
\]
Then $\eta = 1$ in $N^{m-3}(S_j)$, $\eta = 0$ in $\Omega \setminus N^{m-2}(S_j)$ and $0 \leq \eta \leq 1$ in $N^{m-2}(S_j) \setminus N^{m-3}(S_j)$. Furthermore, $H\|\nabla \eta\|_{\infty} \leq \gamma$ and supp$(\nabla \eta) = N^{m-2}(S_j) \setminus N^{m-3}(S_j)$. Take $w = \eta \tilde{\psi}_j - I^{-1}_{H,loc}(H(\eta \tilde{\psi}_j)) \in W(N^m(S_j))$. Then, we can prove that

$$\| \nabla (\psi_j - \psi_{j,loc,m}) \| = \| \nabla (\tilde{\psi}_j - \psi_{j,loc,m}) \| \leq C\| \nabla (\tilde{\psi}_j - w) \| \leq C\varepsilon^{-2}\| \tilde{\psi}_j - w \|_e^2$$

$$\leq C\left(\| \nabla ((1 - \eta)\tilde{\psi}_j) \| + \frac{1}{\varepsilon^2}\| (1 - \eta)\tilde{\psi}_j \| \right)$$

$$+ \| \nabla (\eta \tilde{\psi}_j) \|^2_{V,Nm(S_j)\setminus N^{m-5}(S_j)} + \frac{1}{\varepsilon^2}\| \eta \tilde{\psi}_j \|^2_{\Psi,Nm(S_j)\setminus N^{m-5}(S_j)}$$

$$\leq C \left(1 + \frac{H^2}{\varepsilon^2} + H^2\| \nabla \eta \|^2_{\infty} \right) \| \nabla \psi_j \|^2_{V,Nm-5(S_j)} + C\frac{H^2}{\varepsilon^2}\| \nabla \psi_j \|^2_{\Omega,Nm-6(S_j)}$$

$$\leq C\| \nabla \psi_j \|^2_{\Omega,Nm-6(S_j)}.$$

(3.38) which completes the proof with Theorem 3.2 and Lemma 3.5.

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

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

(3.39)

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

$$\|v_1 - v_2\| \leq C\varepsilon\| \nabla (v_1 - v_2) \| \leq C\varepsilon\sum_{k=1}^{N_H} \|(v, \phi_k)\| \| \nabla (\psi_k - \psi_{k,loc,m}) \|$$

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

(3.40) 

**Lemma 3.8.** The Galerkin approximation of (2.5) in $\Psi_{H,m}$ is to seek $u_{H,m} \in \Psi_{H,m}$ such that

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

(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 oversampling size $m$ satisfies

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

(3.42)

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

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

**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

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

(3.43)
\[ ||u - u_{H,m}|| \leq C \frac{H^2}{\varepsilon^2} ||f||. \] (3.44)

Moreover, if \( f \in H^1(\Omega) \), then
\[ ||u - u_{H,m}||_e \leq C \frac{H^2}{\varepsilon} ||f||_{H^1}, \] (3.45)
\[ ||u - u_{H,m}|| \leq C \frac{H^3}{\varepsilon^2} ||f||_{H^1}. \] (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
\[ ||u - u_{H,m}||_e \leq ||u - \tilde{u}_{H,m}||_e. \] (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
\[
||u - \tilde{u}_{H,m}||_e^2 = a(u - \tilde{u}_{H,m}, u - \tilde{u}_{H,m}) = a(u, u - \tilde{u}_{H,m}) + a(u_H - \tilde{u}_{H,m}, u - \tilde{u}_{H,m}) \\
\leq C H ||f||_e ||\nabla(u - \tilde{u}_{H,m})||_e + ||u_H - \tilde{u}_{H,m}||_e ||u - \tilde{u}_{H,m}||_e \\
\leq C \frac{H}{\varepsilon} ||f||_e ||u - \tilde{u}_{H,m}||_e + C \varepsilon H^{-\frac{3d}{2}} |\beta^m||u||_e ||u - \tilde{u}_{H,m}||_e \\
\leq C \frac{H}{\varepsilon} ||f||_e ||u - \tilde{u}_{H,m}||_e + C \varepsilon H^{-\frac{3d}{2}} C_{\text{st}}(\varepsilon, V) \beta^m ||f||_e ||u - \tilde{u}_{H,m}||_e. \] (3.48)

Hence if \( m \) satisfies Assumption 3.2, then
\[ ||u - u_{H,m}||_e \leq C \frac{H}{\varepsilon} ||f||_e. \] (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 2.2 that
\[
||u - \tilde{u}_{H,m}||_e^2 = (f, u - \tilde{u}_{H,m}) + a(u_H - \tilde{u}_{H,m}, u - \tilde{u}_{H,m}) \\
\leq C \frac{H^2}{\varepsilon} ||\nabla f||_e ||u - \tilde{u}_{H,m}||_e + C \varepsilon H^{-\frac{3d}{2}} |\beta^m||f||_e ||u - \tilde{u}_{H,m}||_e. \] (3.50)

Hence if \( m \) satisfies Assumption 3.2, we can obtain
\[ ||u - u_{H,m}||_e \leq C \frac{H^2}{\varepsilon} ||f||_{H^1}. \] (3.51)

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

**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 OC MsFEM for the Schrödinger equation \((2.1)\), where the Crank-Nicolson scheme is used for temporal discretization. Throughout this section, we will not distinguish between the global multiscale finite element space \(\Psi_H\) 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 \(\Psi_H\).

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 \(\Psi_H\) such that \(\forall 0 \leq t \leq T, \hat{u}(t) \in \Psi_H\) 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 that for any \(0 \leq t \leq T\)

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

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

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

**Proof.** We first consider the case where \(u_t(t) \in L^2(\Omega), \forall t \in [0, T]\). By \((2.1)\), Theorem 3.1, Theorem 3.3 and Lemma 2.3, we have that for any \(0 \leq t \leq T\),

\[
||u(t) - \hat{u}(t)||_e \leq C\frac{H}{\varepsilon}||Hu(t)|| \leq CH||u_t(t)|| \leq C\frac{H}{\varepsilon}, \tag{4.4}
\]

\[
||u(t) - \hat{u}(t)|| \leq C\frac{H^2}{\varepsilon^2}||Hu(t)|| \leq C\frac{H^2}{\varepsilon}||u_t(t)|| \leq C\frac{H^2}{\varepsilon^2}. \tag{4.5}
\]

Moreover, if \(u_t(t) \in H^1(\Omega)\) for any \(t \in [0, T]\), by \((2.1)\), Theorem 3.1, Theorem 3.3, Lemma 2.3, and Lemma 2.5, we know that for any \(0 \leq t \leq T\),

\[
||u(t) - \hat{u}(t)||_e \leq C\frac{H^2}{\varepsilon}||Hu(t)||_{H^1} \leq CH^2||u_t(t)||_{H^1} \leq C\frac{H^2}{\varepsilon^2\delta}, \tag{4.6}
\]

\[
||u(t) - \hat{u}(t)|| \leq C\frac{H^3}{\varepsilon^2}||Hu(t)||_{H^1} \leq C\frac{H^3}{\varepsilon}||u_t(t)||_{H^1} \leq C\frac{H^3}{\varepsilon^3\delta}. \tag{4.7}
\]

\[\blacksquare\]

**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 that for any \(0 \leq t \leq T\)

\[
||\partial_t^k u(t) - \partial_t^k \hat{u}(t)||_e \leq \frac{CH}{\varepsilon^{1-k}\min\{\varepsilon^{2k}, \delta^{2k}\}}, \quad ||\partial_t^k u(t) - \partial_t^k \hat{u}(t)|| \leq \frac{CH^2}{\varepsilon^{2-k}\min\{\varepsilon^{2k}, \delta^{2k}\}}. \tag{4.8}
\]
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 that for any $0 \leq t \leq T$

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

The proof of Lemma 4.2 is similar to Lemma 4.1. We can easily see that higher regularity of the solution $u$ will lead to super convergence of the projection errors in $\Psi_H$ w.r.t. $H$.

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

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

Then

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

Let $\chi(t)$ be the interpolation of $u(t)$ in $\Phi_H$ such that $\chi = \sum_{x_k \in N_H} u(t, x_k) \phi_k$, where $\phi_j(x_k) = \delta_{j,k}$. A well known result for the errors of the interpolation [2, 6, 41] is that

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

and hence

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

By Lemma 2.4 and under Assumption 3.1, we know that for any $0 \leq t \leq T$,

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

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

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

In comparison with Lemma 4.1, we find that the projection error estimate of the OC MsFEM depends on higher temporal regularity of the solution $u$, while that of FEM depends on higher spatial regularity of $u$. Lemmas 2.3, 2.4 and 2.5 show that in the presence of the multiscale potential $V^\delta$, 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 the FEM in solving Schrödinger equation with multiscale potentials due to its super convergence behavior for high-regularity solutions and weaker dependence on the small parameters $\varepsilon$ and $\delta$ for low-regularity solutions.

4.2. Crank-Nicolson OC MsFEM scheme

We analyse the error estimate of the Crank-Nicolson OC MsFEM scheme for (2.1), where we use the Crank-Nicolson scheme in temporal discretization and the OC MsFEM in spatial
Moreover, in the following, we introduce some notations. For some \( N \in \mathbb{N} \) and \( N > 0 \), let \( \Delta t = \frac{T}{N} \) and \( t_n = n\Delta t, n = 0, 1, \ldots, N \).

We approximate \( u(t_n) \) by \( U^n \in \Psi_H \) such that
\[
i\varepsilon(\bar{\partial}U^n, w) = a\left(\frac{U^n + U^{n-1}}{2}, w\right), \quad \forall w \in \Psi_H, n = 1, \ldots, N,
\]
(4.16)
\[
U^0 = \hat{u}(0),
\]
where \( \bar{\partial}U^n = \frac{U^n - U^{n-1}}{\Delta t} \). We 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, \( \theta^n \) satisfies that \( \theta^0 = 0 \) and
\[
i\varepsilon(\bar{\partial}\theta^n, w) + i\varepsilon(z_1^n, w) + i\varepsilon(z_2^n, w) = a\left(\frac{\theta^n + \theta^{n-1}}{2}, w\right), \quad \forall w \in \Psi_H, \quad n = 1, \ldots, N,
\]
(4.17)
where \( \bar{\partial}\theta^n = \frac{\theta^n - \theta^{n-1}}{\Delta t} \), \( z_1^n = \bar{\partial}\hat{u}(t_n) - \bar{\partial}u(t_n) \) and \( z_2^n = \bar{\partial}u(t_n) - \frac{u(t_n) + u(t_{n-1})}{2} \) with \( \bar{\partial}\hat{u}(t_n) = \frac{\hat{u}(t_n) - \hat{u}(t_{n-1})}{\Delta t} \).

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

**Theorem 4.1.** Assume that \( U^N \) is the solution of (4.16) 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
\[
||U^N - u(T)|| \leq C \left( \frac{\varepsilon \Delta t^2}{\min\{\varepsilon^4, \delta^4\}} + \frac{H^2}{\varepsilon \min\{\varepsilon^2, \delta^2\}} \right).
\]
(4.18)
Moreover, if \( u_t(t), u_{tt}(t) \in H^1(\Omega) \) for any \( t \in [0, T] \), then
\[
||U^N - u(T)|| \leq C \left( \frac{\varepsilon \Delta t^2}{\min\{\varepsilon^4, \delta^4\}} + \frac{H^3}{\varepsilon^2 \delta \min\{\varepsilon^2, \delta^2\}} \right).
\]
(4.19)

**Proof.** We 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
\[
||U^N - u(t_n)|| \leq ||\theta^n|| + ||\rho^n|| \quad \text{and} \quad ||\rho^N|| \leq \frac{C H^2}{\varepsilon^2}, \theta^0 = 0.
\]
Setting \( w = \theta^n + \theta^{n-1} \) in (4.17) and taking the imaginary part of it, we have
\[
\text{Re}(\bar{\partial}\theta^n, \theta^n + \theta^{n-1}) = -\text{Re}(z_1^n + z_2^n, \theta^n + \theta^{n-1}),
\]
which implies
\[
\frac{1}{\Delta t}(||\theta^n||^2 - ||\theta^{n-1}||^2) \leq (||\theta^n|| + ||\theta^{n-1}||)(||z_1^n|| + ||z_2^n||).
\]
(4.20)
Therefore, we have
\[
||\theta^N|| \leq ||\theta^0|| + \Delta t \sum_{n=1}^{N}(||z_1^n|| + ||z_2^n||).
\]
(4.21)
For \( ||z_1^n||, n = 1, 2, \ldots, N, \)
\[
||z_1^n|| = ||\bar{\partial}\hat{u}(t_n) - \bar{\partial}u(t_n)|| \leq \frac{1}{\Delta t} \int_{t_{n-1}}^{t_n} ||\hat{u}(s) - u_t(s)|| ds
\]
\[
\leq \frac{C H^2}{\varepsilon} \int_{t_{n-1}}^{t_n} ||u_{tt}(s)|| ds \leq \frac{C H^2}{\varepsilon \min\{\varepsilon^2, \delta^2\}}.
\]
(4.22)
This gives us that $\Delta t \sum_{n=1}^{N} ||z_n|| \leq \frac{C H^2}{\min\{\varepsilon^2, \delta^2\}^2}$. For $||z_n||$, $n = 1, 2, \ldots, N$, we have
\[
||z_2|| = \frac{1}{2\Delta t} ||2(u(t_n) - u(t_{n-1})) - \Delta t(u_t(t_n) + u_t(t_{n-1}))|| \\
\leq \frac{1}{2\Delta t} \left( \int_{t_{n-1}}^{t_n} (t_n - s)^2 ||u_{ttt}(s)||ds + \int_{t_{n-1}}^{t_{n-\frac{1}{2}}} (s - t_{n-1})^2 ||u_{ttt}(s)||ds \right) \\
+ \Delta t \int_{t_{n-\frac{1}{2}}}^{t_n} (t_n - s)||u_{ttt}(s)||ds + \Delta t \int_{t_{n-1}}^{t_{n-\frac{1}{2}}} (s - t_{n-1})||u_{ttt}(s)||ds \\
\leq C \Delta t^2 \max_{0 \leq t \leq T} ||u_{ttt}(t)|| \leq \frac{C \varepsilon \Delta t^2}{\min\{\varepsilon^4, \delta^4\}}, \tag{4.23}
\]
and hence $\Delta t \sum_{n=1}^{N} ||z_n|| \leq \frac{C \varepsilon \Delta t^2}{\min\{\varepsilon^4, \delta^4\}}$. Combining all the above inequalities, we obtain
\[
||U^N - u(T)|| \leq C \left( \frac{\varepsilon \Delta t^2}{\min\{\varepsilon^4, \delta^4\}} + \frac{H^2}{\varepsilon \min\{\varepsilon^2, \delta^2\}} \right). \tag{4.24}
\]
Moreover, if $u_t(t), u_{tt}(t) \in H^1(\Omega)$ for any $t \in [0, T]$, then we have $||\rho^N|| \leq C \frac{H^3}{\varepsilon \delta}$ and for $n = 1, 2, \ldots, N$,
\[
||z_n^N|| \leq \frac{C}{\Delta t} \frac{H^3}{\varepsilon} \int_{t_{n-1}}^{t_n} ||u_{ttt}(s)||_{H^1}ds \leq \frac{C H^3}{\varepsilon \delta \min\{\varepsilon^2, \delta^2\}} \tag{4.25}
\]
Using similar arguments, we can prove the estimate in (4.19).
\[\square\]

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

**Theorem 4.2.** Assume that $U^N$ is the solution of (4.16) 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
\[
||U^N - u(T)||_{e} \leq C \left( \frac{H}{\varepsilon} + \frac{H^2}{\min\{\varepsilon^3, \delta^3\}} + \frac{\varepsilon^2 \Delta t^2}{\min\{\varepsilon^5, \delta^5\}} \right). \tag{4.26}
\]
Moreover, if $u_t(t), u_{tt}(t), u_{ttt}(t) \in H^1(\Omega)$ for any $t \in [0, T]$, then
\[
||U^N - u(T)||_{e} \leq C \left( \frac{H^2}{\varepsilon \delta} + \frac{H^3}{\varepsilon \delta \min\{\varepsilon^3, \delta^3\}} + \frac{\varepsilon^2 \Delta t^2}{\min\{\varepsilon^5, \delta^5\}} \right). \tag{4.27}
\]

**Proof.** We 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 $||U^n - u(t_n)||_e \leq ||\theta^n||_e + ||\rho^n||_e$, where $||\rho^n||_e \leq C \frac{H}{\varepsilon}$. Setting $w = \theta^n - \theta^{n-1}$ in (4.17) and taking the real part of it, we have
\[
||\theta^n||_e^2 \leq ||\theta^{n-1}||^2_e + 2\varepsilon ||z_1^n + z_2^n, \theta^n - \theta^{n-1}|| \leq ||\theta^{n-1}||^2_e + 2\varepsilon ||\theta^n - \theta^{n-1}||^2_e + 2\varepsilon ||z_1^n|| + ||z_2^n||. \tag{4.28}
\]
For $||\theta^n - \theta^{n-1}||$, we can derive by (4.17) that
\[
i\varepsilon(\bar{\partial}\theta^n - \bar{\partial}\theta^{n-1}, w) + i\varepsilon(z_1^n - z_1^{n-1}, w) + i\varepsilon(z_2^n - z_2^{n-1}, w) = a \left( \frac{\theta^n - \theta^{n-2}}{2}, w \right), \quad \forall w \in \Psi_H. \tag{4.29}
\]

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

$$||\bar{\partial}^n||^2 - ||\partial^{n-1}||^2 \leq (||\bar{\partial}^n|| + ||\partial^{n-1}||)(||z^1_n - z^{n-1}_1|| + ||z^n_2 - z^{n-1}_2||)$$  \hspace{1cm} (4.30)

and hence

$$||\theta^n - \theta^{n-1}|| \leq ||\theta^1 - \theta^0|| + \Delta t \sum_{j=2}^{n} (||z^j - z^{j-1}|| + ||z^n_j - z^{n-1}_j||).$$ \hspace{1cm} (4.31)

For $||\theta^1 - \theta^0||$, we have by the proof of Theorem 4.1 that

$$||\theta^1 - \theta^0|| = ||\theta^1|| \leq \Delta t(||z^1_1|| + ||z^n_2||) \leq C \left( \frac{\varepsilon \Delta t^3}{\min\{\varepsilon^4, \delta^4\}} + \frac{\Delta t H^2}{\varepsilon \min\{\varepsilon^2, \delta^2\}} \right),$$ \hspace{1cm} (4.32)

For $\Delta t \sum_{j=2}^{n} ||z^j - z^{j-1}||$, we have

$$||z^j_1 - z^{j-1}_1|| = \frac{1}{\Delta t} ||\rho(t_j) - 2\rho(t_{j-1}) + \rho(t_{j-2})|| \leq \frac{1}{\Delta t} \left( \int_{t_{j-1}}^{t_j} (t_j - s)||\rho_{tt}(s)||ds + \int_{t_{j-2}}^{t_{j-1}} (s - t_{j-2})||\rho_{tt}(s)||ds \right) \leq C \frac{\Delta t H^2}{\varepsilon \min\{\varepsilon^4, \delta^4\}} \max_{0 \leq t \leq T} ||u_{ttt}(t)|| \leq C \frac{\Delta t H^2}{\varepsilon \min\{\varepsilon^4, \delta^4\}} \hspace{1cm} (4.33)

and hence $\Delta t \sum_{j=2}^{n} ||z^j - z^{j-1}|| \leq \frac{C \Delta t H^2}{\min\{\varepsilon^4, \delta^4\}}$. For the term $\Delta t \sum_{j=2}^{n} ||z^j_2 - z^{j-1}_2||$, we have

$$||z^j_2 - z^{j-1}_2|| = \frac{1}{2\Delta t} ||2(u(t_j) - 2u(t_{j-1}) + u(t_{j-2})) - \Delta t(u_{tt}(t_j) - u_{tt}(t_{j-2}))|| \leq \frac{1}{2\Delta t} \left( \int_{t_{j-1}}^{t_j} (t_j - s)^2||u_{ttt}(s)||ds + 2 \int_{t_{j-2}}^{t_{j-1}} (s - t_{j-2})^2||u_{ttt}(s)||ds + 3\Delta t \int_{t_{j-1}}^{t_j} (t_j - s)^2||u_{ttt}(s)||ds + 3\Delta t \int_{t_{j-2}}^{t_{j-1}} (s - t_{j-2})^2||u_{ttt}(s)||ds \right) \leq C \frac{\varepsilon \leq \Delta t^3}{\min\{\varepsilon^6, \delta^6\}} \hspace{1cm} (4.34)

and hence $\Delta t \sum_{j=2}^{n} ||z^j_2 - z^{j-1}_2|| \leq \frac{C \varepsilon \leq \Delta t^3}{\min\{\varepsilon^6, \delta^6\}}$. Therefore

$$||\theta^n||_e^2 \leq ||\theta^0||_e^2 + C\varepsilon \left( \frac{\Delta t H^2}{\min\{\varepsilon^4, \delta^4\}} + \frac{\varepsilon \leq \Delta t^3}{\min\{\varepsilon^6, \delta^6\}} \right) \sum_{n=1}^{N} (||z^n_1|| + ||z^n_2||).$$ \hspace{1cm} (4.35)

According to the proof of Theorem 4.1, we have $\Delta t \sum_{n=1}^{N} ||z^n_1|| \leq \frac{CH^2}{\varepsilon \min\{\varepsilon^2, \delta^2\}}$ and $\Delta t \sum_{n=1}^{N} ||z^n_2|| \leq \frac{C \varepsilon \leq \Delta t^2}{\min\{\varepsilon^4, \delta^4\}}$. Therefore, we obtain

$$||U^n - u(T)||_e \leq C \left( \frac{H}{\varepsilon} + \frac{H^2}{\min\{\varepsilon^2, \delta^2\}} + \frac{\varepsilon \leq \Delta t^2}{\min\{\varepsilon^5, \delta^5\}} \right).$$ \hspace{1cm} (4.36)
Moreover, if \( u_t(t), u_{tt}(t), u_{ttt}(t) \in H^1(\Omega) \) for any \( t \in [0, T] \), then we have \( \|\rho^N\|_e \leq C \frac{H^2}{\varepsilon^3} \) and for \( j = 2, 3, \ldots, N \),

\[
\|z^j_1 - z^{j-1}_1\| \leq C \frac{\Delta t H^3}{\varepsilon} \max_{0 \leq t \leq T} \|u_{ttt}(t)\|_{H^1} \leq \frac{C \Delta t H^3}{\varepsilon \delta \min\{\varepsilon^3, \delta^4\}}. \tag{4.37}
\]

And from the proof of Theorem 4.1, we know that

\[
\|\theta^1 - \theta^0\| \leq C \left( \frac{\varepsilon \Delta t^3}{\min\{\varepsilon^4, \delta^4\}} + \frac{\Delta t H^3}{\varepsilon^2 \delta \min\{\varepsilon^2, \delta^2\}} \right), \quad \Delta t \sum_{n=1}^{N} \|z^n_1\| \leq \frac{C H^3}{\varepsilon^2 \delta \min\{\varepsilon^2, \delta^2\}}. \tag{4.38}
\]

Hence we can obtain the estimate (4.27) using similar arguments.

**Remark 4.1.** For the estimates in Theorem 4.1, and Theorem 4.2, the constants \( C \)'s depend polynomially and at most quadratically on the final time \( T \).

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 \( \Omega = [0, 2\pi] \), final time \( T = 0.5 \) and initial data

\[
u_0(x) = \left( \frac{10}{\pi} \right)^{1/4} \exp \left( -5(x - \pi)^2 \right) \exp \left( -i \frac{(x - \pi)^2}{\varepsilon} \right). \tag{5.1}
\]

We will compare the relative errors between the numerical solution \( u_{\text{num}} \) and the reference solution \( u_{\text{ref}} \) in \( L^2 \) norm and \( H^1 \) norm with

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

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 \( \Delta t = \frac{1}{2\pi}, H = \frac{\pi}{2\pi} \). The numerical solution is computed by the Crank-Nicolson standard linear FEM and the Crank-Nicolson localized OC MsFEM with \( \Delta t = \frac{1}{24} \) and \( H = \frac{\pi}{24}, \frac{\pi}{96}, \frac{\pi}{192}, \frac{\pi}{384}, \frac{\pi}{768} \) for case (i), \( H = \frac{\pi}{24}, \frac{\pi}{192}, \frac{\pi}{384}, \frac{\pi}{768}, \frac{\pi}{1536}, \frac{\pi}{3072} \) for case (ii). The oversampling size for the localized OC MsFEM is chosen as \( m = 3 \lceil \log_2(2/\eta) \rceil \). The results are shown in Table 1, Table 2, Figure 1, and Figure 2.
Table 1: Errors for potential (5.3) with $\varepsilon = 1/8$ and $\delta = 1/10$.

| $H$ | $\pi/64$ | $\pi/128$ | $\pi/256$ | $\pi/512$ | $\pi/1024$ |
|-----|----------|-----------|------------|-----------|------------|
| $\text{err}_{L^2}$ of FEM | 1.0609E-01 | 4.9109E-02 | 2.8067E-02 | 1.2637E-02 | 7.1021E-03 |
| convergence order | 1.90 | 1.94 | 1.83 | 2.24 |
| $\text{err}_{L^2}$ of localized OC MsFEM | 2.7487E-04 | 3.8263E-05 | 1.1229E-05 | 2.1894E-06 | 8.0399E-07 |
| convergence order | 4.86 | 4.26 | 3.75 | 3.90 |
| $\text{err}_{H^1}$ of FEM | 2.7651E-01 | 1.4938E-01 | 9.9142E-02 | 5.8818E-02 | 4.1849E-02 |
| convergence order | 1.52 | 1.43 | 1.20 | 1.32 |
| $\text{err}_{H^1}$ of localized OC MsFEM | 3.6524E-03 | 9.8017E-04 | 4.0261E-04 | 1.1748E-04 | 4.8910E-05 |
| convergence order | 3.24 | 3.09 | 2.82 | 3.41 |

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

| $H$ | $\pi/128$ | $\pi/256$ | $\pi/512$ | $\pi/1024$ | $\pi/2048$ |
|-----|-----------|-----------|------------|-----------|------------|
| $\text{err}_{L^2}$ of FEM | 1.0269E+00 | 7.6698E-01 | 4.4394E-01 | 2.7804E-01 | 1.3189E-01 |
| convergence order | 1.01 | 1.25 | 1.82 | 1.71 |
| $\text{err}_{L^2}$ of localized OC MsFEM | 1.3898E-01 | 2.7714E-02 | 1.8745E-03 | 3.2749E-04 | 4.9916E-05 |
| convergence order | 5.60 | 6.17 | 6.79 | 4.31 |
| $\text{err}_{H^1}$ of FEM | 1.3217E+00 | 1.0963E+00 | 7.1925E-01 | 4.9949E-01 | 2.6246E-01 |
| convergence order | 0.65 | 0.97 | 1.42 | 1.48 |
| $\text{err}_{H^1}$ of localized OC MsFEM | 3.0094E-01 | 7.7003E-02 | 1.0450E-02 | 3.6681E-03 | 9.8675E-04 |
| convergence order | 4.47 | 4.58 | 4.08 | 3.01 |

Figure 1: Errors for potential (5.3) with $\varepsilon = 1/8$ and $\delta = 1/10$.
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 (4.19), (4.27) proposed in Theorem 4.1 and Theorem 4.2. This super-convergence behavior is due to the smoothness of the potential (5.3) that results in a solution with high regularity.

5.2. Discontinuous Potentials

Consider the potential

$$V = |x - \pi|^2 + 2 + \begin{cases} \cos \left( \frac{x}{\delta_1} \right), & x \in [0, \pi], \\ \cos \left( \frac{x}{\delta_2} \right), & x \in (\pi, 2\pi]. \end{cases}$$ (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 $\Delta t = \frac{1}{20\pi}, H = \frac{\pi}{1024}$. The numerical solutions are computed by the time-splitting spectral method (TSSP), Crank-Nicolson standard linear FEM and Crank-Nicolson localized OC MsFEM with $\Delta t = \frac{1}{24}$ 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 $m = 2 \lceil \log_2(\frac{2\pi}{H}) \rceil$. The results are shown in Table 3, Table 4, Figure 3, and Figure 4.
Table 3: Errors for potential (5.4) with $\varepsilon = 1/8$, $\delta_1 = 1/5$, and $\delta_2 = 1/10$.

| $H$          | $\pi^{64}$ | $\pi^{96}$ | $\pi^{128}$ | $\pi^{192}$ | $\pi^{256}$ |
|-------------|------------|------------|------------|------------|------------|
| $\text{err}_{L^2}$ of TSSP | 4.1036E-01 | 2.6171E-01 | 2.0189E-01 | 1.1358E-01 | 9.9578E-02 |
| convergence order | 1.11 | 0.90 | 1.32 | 0.51 | |
| $\text{err}_{L^2}$ of FEM | 1.2790E-01 | 6.8296E-02 | 4.4099E-02 | 2.4116E-02 | 1.5917E-02 |
| convergence order | 1.55 | 1.52 | 1.38 | 1.62 | |
| $\text{err}_{L^2}$ of localized OC MsFEM | 8.8626E-03 | 4.0528E-03 | 2.3565E-03 | 1.1604E-03 | 6.4039E-04 |
| convergence order | 1.93 | 1.88 | 1.62 | 2.31 | |
| $\text{err}_{H^1}$ of TSSP | 5.1651E-01 | 3.2669E-01 | 2.5942E-01 | 1.4208E-01 | 1.2934E-01 |
| convergence order | 1.13 | 0.80 | 1.38 | 0.37 | |
| $\text{err}_{H^1}$ of FEM | 3.3974E-01 | 2.2411E-01 | 1.7045E-01 | 1.1976E-01 | 9.5007E-02 |
| convergence order | 1.03 | 0.95 | 0.81 | 0.90 | |
| $\text{err}_{H^1}$ of localized OC MsFEM | 5.7921E-02 | 4.3351E-02 | 3.2635E-02 | 2.2383E-02 | 1.5132E-02 |
| convergence order | 0.71 | 0.99 | 0.86 | 1.52 | |

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

| $H$          | $\pi^{96}$ | $\pi^{128}$ | $\pi^{192}$ | $\pi^{256}$ | $\pi^{384}$ |
|-------------|------------|------------|------------|------------|------------|
| $\text{err}_{L^2}$ of TSSP | 8.6933E-01 | 8.2000E-01 | 7.2275E-01 | 5.1762E-01 | 4.7231E-01 |
| convergence order | 0.20 | 0.29 | 1.30 | 0.21 | |
| $\text{err}_{L^2}$ of FEM | 1.0980E+00 | 8.2753E-01 | 4.9740E-01 | 3.2823E-01 | 1.6666E-01 |
| convergence order | 0.98 | 1.17 | 1.62 | 1.55 | |
| $\text{err}_{L^2}$ of localized OC MsFEM | 1.8558E-01 | 5.9763E-02 | 1.4948E-02 | 7.0768E-03 | 2.7845E-03 |
| convergence order | 3.94 | 3.18 | 2.91 | 2.14 | |
| $\text{err}_{H^1}$ of TSSP | 9.4843E-01 | 8.6754E-01 | 6.5087E-01 | 5.2097E-01 | 6.0281E-01 |
| convergence order | 0.31 | 0.66 | 0.87 | -0.33 | |
| $\text{err}_{H^1}$ of FEM | 1.1400E+00 | 9.5249E-01 | 6.7419E-01 | 4.8814E-01 | 2.9260E-01 |
| convergence order | 0.62 | 0.79 | 1.26 | 1.17 | |
| $\text{err}_{H^1}$ of localized OC MsFEM | 3.1450E-01 | 1.3862E-01 | 5.3020E-02 | 3.2920E-02 | 2.2157E-02 |
| convergence order | 2.85 | 2.20 | 1.85 | 0.91 | |
The time-splitting spectral method suffers from reduced convergence order and low accuracy due to the discontinuous potential (5.4). However, convergence rates of approximately 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 due to the fact that for a solution with low regularity in the presence of a multiscale potential, the projection error estimates of the OC MsFEM depend more weakly on the small parameters than the FEM. The result is consistent with the discussion in Section 4.1. This numerical example shows that the OC MsFEM is robust in the sense that it still yields an accurate solution for the semiclassical Schrödinger equation with a discontinuous multiscale potential.

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 general 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. By combining the analysis on the regularity of the solution, we also derive the dependence of the error estimates on the small parameters. 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 for high-regularity solutions and weaker dependence on the small parameters $\varepsilon$ and $\delta$ for low-regularity solutions. The weaker dependence of the OC MsFEM on the small parameters is a consequence of the fact that the time derivatives of the solution are less oscillatory than the spatial derivatives in the presence of the multiscale potential. 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 semiclassical 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 the semiclassical regime. 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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