COMMUN. MATH. SCI.
Vol. 18, No. 3, pp. 687–706

EXTENDED WKB ANALYSIS FOR THE LINEAR VECTORIAL WAVE EQUATION IN THE HIGH-FREQUENCY REGIME*

CHUNXIONG ZHENG† AND JIASHUN HU‡

Abstract. We introduce an asymptotic solution form, termed as *extended Wentzel-Kramers-Brillouin* (E-WKB), to solve the high-frequency vectorial wave equation when the initial Cauchy data are prescribed in the form of Wentzel-Kramers-Brillouin (WKB) function. The E-WKB form, formulated as an integral of a family of Gaussian coherent states, can be regarded as an extension of the WKB form. The domain of the integral is the Lagrangian submanifold induced by the underlying Hamiltonian flow. Although the procedure of solving wave equations by using the E-WKB form is parallel to that of the classical WKB analysis, the former can overcome the difficulty due to the presence of caustic points. We present numerical tests on vectorial Schrödinger equation and Helmholtz equation to validate the proposed asymptotic theory.

Keywords. Vectorial wave equation; high-frequency regime; caustics; WKB analysis; extended WKB analysis.

AMS subject classifications. 34E20; 35S10; 35C20.

1. Introduction

Wave propagation is a classical problem in physics and mathematics. For wave equations with high-frequency characteristics, the geometrical optics method presents us asymptotic solutions. This method assumes the solution u to admit the Wentzel-Kramers-Brillouin (WKB) ansatz, see [1]:

$$u(x)=A^{\varepsilon}\exp[\mathrm{i}S(x)/\varepsilon],\ A^{\varepsilon}=\sum_{j=0}^{\infty}(-\mathrm{i}\varepsilon)^{j}A_{j}.$$

In the WKB form, ε is the reverse of the high frequency, S is a smooth real function called phase, and $\{A_j\}_{j=0}^{\infty}$ is a sequence of smooth functions called amplitudes which do not depend on the small asymptotic parameter ε. By substituting the ansatz into the high-frequency equation and cancelling the exponential term, it allows us to obtain a system of equations for S and A_j. The asymptotic approximation is then obtained by solving the derived equation system.

In many situations, however, the phase S is not uniquely determined around the caustic points, which leads to the well-known caustic problem when applying the WKB method to the governing equation. Mathematically, the caustic problem arises from the singularities of parametrization of the associated Lagrangian submanifold, which can be solved by the canonical operator method developed by Maslov [2]. In Maslov's method, several local charts of the Lagrangian submanifold are chosen to ensure that the submanifold can be represented as a graph manifold in Lagrangian coordinates. Then local asymptotic solutions are constructed by employing WKB method in these local charts. With the help of the Maslov index, local asymptotic solutions are assembled to provide a global approximation. However, this method requires us to set up a specific

*Received: November 18, 2018; Accepted (in revised form): November 18, 2019. Communicated by Shi Jin.

†College of Mathematics and Systems Science, Xinjiang University, Urumqi, 830046, P.R. China; and Department of Mathematical Sciences, Tsinghua University, Beijing, 100084, China (czheng@mail.tsinghua.edu.cn).

‡Department of Mathematical Sciences, Tsinghua University, Beijing, 100084, China (hjs16@mails.tsinghua.edu.cn).

partition of the associated Lagrangian submanifold. For high-dimensional problems, this is not an easy task from the numerical point of view.

In 1960s, another semiclassical approximation method, called the Gaussian beam approach, had been developed (see [3]) and later applied to the high-frequency wave equation by Hörmander [4] and Ralston [5]. The Gaussian beam approach can solve the caustic problem without the requirement to set up the partition of the associated Lagrangian submanifold. In recent years, there are many investigations about this method. For example, the Gaussian beam method has been applied to various types of equations in [6, 7], higher order asymptotic solutions are given in [8–10], and the accuracy analysis of this method is discussed in [11–14]. In 2014, Zheng [15] proved the optimal error estimate for the first-order Gaussian beam approximation. The Gaussian beam method can also be used to solve the boundary value problem of high-frequency wave, see [16, 17]. For more literature on the Gaussian beam method, we refer the readers to the review [18].

The method proposed in this paper is based on another form of solution ansatz which can be regarded as an extension of the WKB form. The proposed asymptotic wave field is defined as an integral of coherent states on a Lagrangian submanifold induced by the Hamiltonian flow. This new ansatz, termed as extended WKB (E-WKB) form, can be applied to scalar equations [19] as well as vectorial equations [20] to obtain approximate solutions even around the caustic points. The key ingredient in those works is called moving-frame technique. Since the caustic problem arises from the choice of singular coordinates, we variate our choice of local coordinates by following a moving frame. Then in each local domain, the phase and amplitude can be uniquely determined by applying the classical WKB analysis to the transformed high-frequency equation in the new coordinate. However, the moving-frame technique tends to be very complicated for the vectorial wave problems, and the results obtained are difficult to generalize.

In this paper, we develop the E-WKB analysis in a way parallel to the classical WKB analysis and recover the results obtained in [19, 20] in a comprehensive way. The motivation lies in that the unknowns are functions defined on the Lagrangian submanifold. Thus we hope to derive the governing equation by directly using differential operations on the corresponding submanifold instead of using local WKB analysis in the moving frame. In order to clarify how the E-WKB analysis works, we first present some key components of the classical WKB analysis and then generalize them to the E-WKB case. Finally we discuss the application of the E-WKB analysis to the linear vectorial wave equation in the high-frequency regime.

The rest of this paper is organized as follows. In Section 2 and Section 3, we introduce some basic notations and recall fundamental material of the classical WKB analysis. In Section 4, we introduce the E-WKB form and generalize the invariance property of the classical WKB form to the E-WKB form. In Section 5 and 6, we work out the governing equations of the phase and the amplitude functions in the vectorial case. In Section 7, we report two numerical tests which both show a first-order accuracy with respect to the asymptotic parameter. We conclude this paper in Section 8.

2. Preliminaries

In this section, we briefly give an introduction to Weyl quantization. We begin with a unitary representation of the Heisenberg group.

2.1. Heisenberg group and its unitary representation. The Heisenberg Lie group $\mathbf{H}_N$ is $\mathbb{R}^{2N}\times\mathbb{R}$ equipped with the group law

$$(z,s)(w,t)=(z+w,s+t+[z,w]/2),\ \forall z,w\in\mathbb{R}^{2N},\ \forall s,t\in\mathbb{R}.$$

The bracket $[\cdot,\cdot]$ refers to the symplectic inner product in $\mathbb{R}^{2N}$, i.e.,

$$[z,w] = q^\dagger u - p^\dagger v = z^\dagger J w,\ z = (q;p),\ w = (v;u),\ \forall q,p,v,u \in \mathbb{R}^N.$$

In the above, $(q;p)$ expresses column vectors in an economical form, and J denotes the standard symplectic matrix, i.e.,

$$(q;p) = \begin{pmatrix} q \\ p \end{pmatrix}, \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

The symbol I stands for the unit matrix, with a dimension generally clearly determined from the context. Here and hereafter, all vectorial objects are arranged in the column form, and we use the symbol † to denote their real transpose. A unitary representation of the Heisenberg group $\mathbf{H}_N$ (scaled by $\varepsilon > 0$) is given by

$$\rho_\varepsilon(z,s) = \exp\{\mathrm{i}([z,W] - s)/\varepsilon\},\ W = (X;\varepsilon D),\ D = -\mathrm{i}\nabla.$$

In the above, X and D denote the position and momentum operators, respectively. Throughout this paper, we make the convention that $\rho_\varepsilon(z) \equiv \rho_\varepsilon(z,0)$. For any $f \in L^2(\mathbb{R}^N)$, it holds that (see page 21 in [21])

$$[\rho_\varepsilon(z) f](x) = \exp\left[-\mathrm{i}p^\dagger (x + q/2)/\varepsilon\right] f(x+q). \tag{2.1}$$

2.2. Weyl quantization. For any proper smooth function $H = H(z)$ defined on the phase space $\mathbb{R}^{2N}$, the symplectic Fourier transform of H is denoted as $\hat{H}$, i.e.,

$$\hat{H}(w) = (2\pi)^{-2N} \int H(z) \exp(\mathrm{i}[z,w])\, dz.$$

The Weyl quantization of H, denoted by $H(W)$, is defined by

$$H(W) = \int \hat{H}(w) \exp(\mathrm{i}[w,W])\, dw = \int \hat{H}(w) \rho_\varepsilon(\varepsilon w) dw. \tag{2.2}$$

It is straightforward to verify that

$$\widehat{\nabla_p H}(w) = \mathrm{i}v \hat{H}(w), \quad \widehat{\nabla_q H}(w) = -\mathrm{i}u \hat{H}(w), \quad w = (v;u),$$

where ∇_q and ∇_p stand for the derivatives with respect to position and momentum variables, respectively. Therefore, given any polynomial function $f(v,u)$, it holds that

$$f(-\mathrm{i}\nabla_p, \mathrm{i}\nabla_q) H(z) = \int_{w=(v;u)} f(v,u) \hat{H}(w) \exp(\mathrm{i}[w,z])\, dw. \tag{2.3}$$

In the language of the Weyl quantization (2.2), in this paper we are concerned with the Cauchy problem of the following general high-frequency vectorial wave equation

$$H(W) u^\varepsilon(x) = 0. \tag{2.4}$$

3. WKB analysis

WKB function is an important concept in the high-frequency asymptotic theory, which gives an intrinsic sparse representation of a highly oscillatory wave field. In this section, we recall some basic elements of the WKB theory. For the sake of generality, we consider the WKB function which takes values in a separated Hilbert space $\mathfrak{H}$.

DEFINITION 3.1. *By an $\mathfrak{H}$-valued WKB function defined on a connected domain $\Omega\subset\mathbb{R}^N$, we mean*

$$\varphi(x)=A^\varepsilon(x)\exp[\mathrm{i}S(x)/\varepsilon] \tag{3.1}$$

with $A^\varepsilon\in C^\infty(\Omega,\mathfrak{H})$ and $S\in C^\infty(\Omega,\mathbb{R})$. Moreover, A^ε admits an asymptotic expansion

$$A^\varepsilon\sim A_0+(-\mathrm{i}\varepsilon)A_1+(-\mathrm{i}\varepsilon)^2A_2+\cdots,$$

where $A_k\in C^\infty(\Omega,\mathfrak{H})$ for all $k\geq 0$.

DEFINITION 3.2. *We define the associated Lagrangian submanifold of the WKB function $\varphi(x)$, see (3.1), as a graph submanifold in the phase space $\mathbb{R}^{2N}$,*

$$\Lambda=\{z=(q;p)\,|\,p=\nabla S(q),\forall q\in\Omega\}. \tag{3.2}$$

The following result plays a key role in the classical geometrical optics. It reveals that the image of a WKB function under the action a Weyl-quantized operator is still a WKB function with variated amplitude function.

THEOREM 3.1. *Suppose that $H=H(z)$ is an operator-valued smooth function acting on a separated Hilbert space $\mathfrak{H}$. For all $A\in C^\infty(\Omega,\mathfrak{H})$, asymptotically it holds that*

$$H(W)A(x)\exp[\mathrm{i}S(x)/\varepsilon]=[T_0A(x)+(-\mathrm{i}\varepsilon)T_1A(x)+\cdots]\exp[\mathrm{i}S(x)/\varepsilon],$$

where $\{T_j\}$ is a sequence of local differential operators acting on $C^\infty(\Omega,\mathfrak{H})$. In particular, the first two operators are given by

$$\begin{aligned}
&T_0A(x)=H(z)A(x),\\
&T_1A(x)=\nabla_pH(z)\cdot\nabla A(x)+\frac{1}{2}\mathrm{tr}\left[\nabla^2S(x)\nabla_p^2H(z)+\nabla_q^\dagger\nabla_pH(z)\right]A(x),
\end{aligned}$$

where $z=(x;\nabla S(x))$.

In order to find an approximate solution $\varphi(x)$ of Equation (2.4) in the WKB form (3.1), we substitute the WKB ansatz $\varphi(x)$ into Equation (2.4) and apply Theorem 3.1 to compute the transformed WKB function. By setting the coefficients of the zeroth- and the first-order terms in ε to be zero, we derive

$$\begin{aligned}
&H(z)A_0(x)=0,\\
&H(z)A_1(x)+T_1A_0(x)=0,
\end{aligned} \tag{3.3}$$

where $z=(x;\nabla S(x))$. The first equation is equivalent to the fact that z lies in the zero level set of some energy surface of $H(z)$ and $A_0(z)$ belongs to the corresponding eigenspace. More precisely, there exists an eigenvalue $\lambda(z)$ of $H(z)$ and its associated eigenspace $E_\lambda(z)$ such that

$$\lambda(z)=0,\quad A_0(x)\in E_\lambda(z),\ \forall z=(x;\nabla S(x)).$$

Now we know that the phase function $S(x)$ satisfies the Hamilton-Jacobi equation:

$$\lambda(x;\nabla S(x))=0. \tag{3.4}$$

Let us assume that the dimension of the eigenspace $E_\lambda(z)$ is a constant κ and $\{b_\beta(z)\}_{\beta=1}^{\kappa}$ forms a smooth basis. Since $A_0(x)\in E_\lambda(z)$, it can be represented as a linear combination of the $b_\beta(z)$, i.e.,

$$A_0(x)=\sum_\beta \sigma^\beta(x)b_\beta(z),$$

where $\{\sigma^\beta(x)\}_{\beta=1}^{\kappa}\subset C^\infty(\mathbb{R}^N,\mathbb{C})$. By introducing the projection $\mathcal{P}(z)$ of $\mathfrak{H}$ onto $E_\lambda(z)$, the Equation (3.3) is simplified to be independent of $A_1(x)$, i.e.,

$$\mathcal{P}(z)T_1A_0(x)=0. \tag{3.5}$$

By representing Equation (3.5) in terms of $\{\sigma^\beta(x)\}_{\beta=1}^{\kappa}$, we obtain:

$$\sum_\beta\left[S_{\alpha,\beta}\cdot\nabla\sigma^\beta(x)+W_{\alpha,\beta}\sigma^\beta(x)+\frac{1}{2}L_{\alpha,\beta}\sigma^\beta(x)\right]=0, \tag{3.6}$$

where

$$\begin{aligned}
&W_{\alpha,\beta}(z)=\langle b_\alpha(z),\nabla_pH(z)\cdot\nabla b_\beta(z)\rangle,\\
&S_{\alpha,\beta}(z)=\langle b_\alpha(z),\nabla_pH(z)b_\beta(z)\rangle,\\
&L_{\alpha,\beta}(z)=\langle b_\alpha(z),\mathrm{tr}\left[\nabla^2S(x)\nabla_p^2H(z)+\nabla_q^\dagger\nabla_pH(z)\right]b_\beta(z)\rangle.
\end{aligned}$$

In the above, the notation $\langle\cdot,\cdot\rangle$ stands for the inner product of the Hilbert space $\mathfrak{H}$. Thus, in principle, we can solve the phase and the leading term of amplitude from (3.4) and (3.6) and obtain an approximate solution in the classical WKB form (3.1).

4. Extended WKB function

In this section, we introduce the concept of E-WKB function, which is a generalization of the classical WKB function. Besides the simple algebraic relation between the components of a WKB function and the related E-WKB function, the importance of the E-WKB function also comes from the fact that the action of a Weyl-quantized operator preserves its form. As we have seen, the invariance property plays an important role in the classical WKB analysis.

DEFINITION 4.1. *Let $\lambda(z)$ be a smooth real-valued function defined in the phase space $\mathbb{R}^{2N}$. By a λ-submanifold Λ, we mean a Lagrangian submanifold generated by continuously displacing a connected isotropic submanifold Λ_{N-1}^I of dimension $N-1$ according to the λ-Hamiltonian vector field. Besides, we assume that Λ is topologically isomorphic to $\Lambda_{N-1}^I\times\mathbb{R}$.*

According to the above definition, Λ can be parameterized as $z=z(z_0;t)$ which obeys the Hamiltonian system

$$\dot z=J\nabla\lambda(z),\quad z(z_0;0)=z_0\in\Lambda_{N-1}^I. \tag{4.1}$$

If the initial isotropic submanifold Λ_{N-1}^I can be parametrized by $(\xi_1,\cdots,\xi_{N-1})$, then the tangent space at $z\in\Lambda$ is represented by a matrix $C\in\mathbb{R}^{2N\times N}$, where

$$C=\left[\frac{\partial z}{\partial\xi_1}\ \cdots\ \frac{\partial z}{\partial\xi_{N-1}}\ \frac{\partial z}{\partial t}\right]. \tag{4.2}$$

DEFINITION 4.2. *We define the ε-scaled fundamental coherent state function of dimension N as*

$$\phi^\varepsilon(x) = (2\pi\varepsilon)^{-N/2} \exp\left(-x^2/2\varepsilon\right).$$

For any $(z,\mathcal{S}) \in \mathbb{R}^{2N} \times \mathbb{R}$ with $z = (q;p)$, the phase space translation of $\phi^\varepsilon(x)$ is defined as

$$\phi^\varepsilon_{z,\mathcal{S}}(x) = \rho_\varepsilon(-z,-\mathcal{S})\phi^\varepsilon(x).$$

From Equation (2.1), we derive the following explicit form

$$\phi^\varepsilon_{z,\mathcal{S}}(x) = (2\pi\varepsilon)^{-N/2} \exp(\mathrm{i}\mathcal{S}/\varepsilon) \exp\left[\mathrm{i}p^\dagger(x-q/2)/\varepsilon\right] \exp\left[-(x-q)^2/2\varepsilon\right].$$

DEFINITION 4.3. *Given a separated Hilbert space $\mathfrak{H}$ and a scalar Hamiltonian $\lambda(z)$, an associated $\mathfrak{H}$-valued E-WKB function is referred to as an integral of the following form*

$$\int_{z=(q;p)\in\Lambda} \mathcal{A}^\varepsilon_z \phi^\varepsilon_{z,\mathcal{S}_z} d\nu_z, \tag{4.3}$$

where Λ is a λ-submanifold, $\mathcal{S}_z \in C^\infty(\Lambda,\mathbb{R})$ is a generating function of the differential 1-form $p^\dagger dq - d(p^\dagger q)/2$ on Λ, and $\mathcal{A}^\varepsilon_z$ admits an asymptotic expansion with respect to ε:

$$\mathcal{A}^\varepsilon_z \sim \mathcal{A}_{0,z} + (-\mathrm{i}\varepsilon)\mathcal{A}_{1,z} + (-\mathrm{i}\varepsilon)^2\mathcal{A}_{2,z} + \cdots,$$

where $\mathcal{A}_{k,z} \in C^\infty(\Lambda,\mathfrak{H})$ for all $k \geq 0$.

The E-WKB function is indeed an extension of the classical WKB function, as is revealed in the following theorem.

THEOREM 4.1. *Given a WKB function*

$$\varphi(x) = A(x) \exp\left[\mathrm{i}S(x)/\varepsilon\right]$$

with A and S defined on a connected domain $\Omega \in \mathbb{R}^N$, and $A \in \mathcal{C}^\infty_0(\Omega)$. Let Λ be the associated Lagrangian submanifold of φ. Then the WKB function φ admits a pointwise E-WKB representation of the following form

$$\varphi(x) = \int_{z=(q;p)\in\Lambda} \mathcal{A}_z \phi^\varepsilon_{z,\mathcal{S}_z}(x) d\nu_z + \mathcal{O}(\varepsilon),$$

where

$$\mathcal{S}_z = S(q) - p^\dagger q/2, \quad \mathcal{A}_z = \det{}^{-\frac{1}{2}}\left[I - \mathrm{i}\nabla^2 S(q)\right] A(q). \tag{4.4}$$

The proof of this theorem can be found in [19].

4.1. Invariance property of E-WKB functions. In this section, we prove the invariance property of the E-WKB form under the action of a Weyl-quantized operator. The key point is to transform the multiplication operation in terms of x to the differential operation in terms of z.

LEMMA 4.1. *Let us denote by $\Pi_z \in \mathbb{R}^{2N\times 2N}$ the projection onto the tangent plane of the Lagrangian submanifold Λ at $z \in \Lambda$. Then for all $z = (q;p) \in \Lambda$, it holds that*

$$(x_k - q_k)\phi^\varepsilon_{z,\mathcal{S}_z}(x) = \mathrm{i}\varepsilon E^\dagger_{z,k} \nabla_\Lambda \phi^\varepsilon_{z,\mathcal{S}_z}(x), \tag{4.5}$$

where ∇_Λ is the gradient operator on Λ and

$$E_{z,k} = \Pi_z \begin{bmatrix} -\mathrm{i}e_k \\ -e_k \end{bmatrix}.$$

In the above, e_k represents the k-th standard basis of $\mathbb{R}^N$.

Proof. Since $d\mathcal{S}_z = p^\dagger dq - d(p^\dagger q)/2$, it is straightforward to verify that

$$\begin{aligned} \mathrm{i}\varepsilon E_{z,k}^\dagger \nabla_\Lambda \phi_{z,\mathcal{S}_z}^\varepsilon &= E_{z,k}^\dagger \Pi_z \begin{bmatrix} \mathrm{i}(x-q) \\ -(x-q) \end{bmatrix} \phi_{z,\mathcal{S}_z}^\varepsilon \\ &= \begin{bmatrix} -\mathrm{i}e_k^\dagger & -e_k^\dagger \end{bmatrix} \Pi_z \begin{bmatrix} \mathrm{i}I \\ -I \end{bmatrix} (x-q)\phi_{z,\mathcal{S}_z}^\varepsilon. \end{aligned}$$

Moreover, from the fact that Λ is a Lagrangian submanifold, it holds that

$$\begin{bmatrix} -\mathrm{i}I & -I \end{bmatrix} \Pi_z \begin{bmatrix} \mathrm{i}I \\ -I \end{bmatrix} = I,$$

which ends the proof. ∎

By iteratively applying the result obtained in Lemma 4.1 and integration by parts, we have the following result.

LEMMA 4.2. *For all $\mathcal{A}_z \in C_0^\infty(\Lambda, \mathfrak{H})$ and all multi-indexes α, it holds that*

$$\int_{z\in\Lambda} (x-q)^\alpha \mathcal{A}_z \phi_{z,\mathcal{S}_z}^\varepsilon d\nu_z = O(\varepsilon^m), \ |\alpha| = 2m-1 \text{ or } 2m.$$

In particular, we have

$$\begin{aligned} &\int_{z\in\Lambda} (x_k - q_k)\mathcal{A}_z \phi_{z,\mathcal{S}_z}^\varepsilon d\nu_z = (-\mathrm{i}\varepsilon)\int_{z\in\Lambda} \mathrm{div}_\Lambda(\mathcal{A}_z E_{z,k})\phi_{z,\mathcal{S}_z}^\varepsilon d\nu_z, \\ &\int_{z\in\Lambda} (x_m - q_m)(x_n - q_n)\mathcal{A}_z \phi_{z,\mathcal{S}_z}^\varepsilon d\nu_z = (-\mathrm{i}\varepsilon)\int_{z\in\Lambda} \mathcal{T}_{z,mn}\mathcal{A}_z \phi_{z,\mathcal{S}_z}^\varepsilon d\nu_z + O(\varepsilon^2), \end{aligned}$$

where

$$\mathcal{T}_{z,mn} = E_{z,m}^\dagger \nabla_\Lambda(-q_n).$$

Proof. By Equation (4.5) and integration by parts, we derive

$$\begin{aligned} \int_{z\in\Lambda} (x_k - q_k)\mathcal{A}_z \phi_{z,\mathcal{S}_z}^\varepsilon d\nu_z &= \mathrm{i}\varepsilon \int_{z\in\Lambda} \mathcal{A}_z E_{z,k}^\dagger \nabla_\Lambda \phi_{z,\mathcal{S}_z}^\varepsilon d\nu_z \\ &= (-\mathrm{i}\varepsilon)\int_{z\in\Lambda} \mathrm{div}_\Lambda(\mathcal{A}_z E_{z,k})\phi_{z,\mathcal{S}_z}^\varepsilon d\nu_z. \end{aligned}$$

Furthermore, it holds that

$$\begin{aligned} &\int_{z\in\Lambda} (x_m - q_m)(x_n - q_n)\mathcal{A}_z \phi_{z,\mathcal{S}_z}^\varepsilon d\nu_z \\ &= (-\mathrm{i}\varepsilon)\int_{z\in\Lambda} \mathrm{div}_\Lambda((x_n - q_n)\mathcal{A}_z E_{z,m})\phi_{z,\mathcal{S}_z}^\varepsilon d\nu_z \end{aligned}$$

$$
\begin{aligned}
&= (-\mathrm{i}\varepsilon)\int_{z\in\Lambda}\left[E_{z,m}^{\dagger}\nabla_{\Lambda}(x_n-q_n)\mathcal{A}_z+(x_n-q_n)\mathrm{div}_{\Lambda}(\mathcal{A}_z E_{z,m})\right]\phi_{z,\mathcal{S}_z}^{\varepsilon}\,d\nu_z \\
&= (-\mathrm{i}\varepsilon)\int_{z\in\Lambda}\mathcal{T}_{z,mn}\mathcal{A}_z\phi_{z,\mathcal{S}_z}^{\varepsilon}\,d\nu_z+O(\varepsilon^2).
\end{aligned}
$$

By induction, for any multi-index α, we have

$$
\int_{z\in\Lambda}\mathcal{A}_z(x-q)^{\alpha}\phi_{z,\mathcal{S}_z}^{\varepsilon}\,d\nu_z=O(\varepsilon^m),\ |\alpha|=2m-1 \text{ or } 2m,
$$

which ends the proof. ∎

Now, we prove the invariance property of the E-WKB function.

THEOREM 4.2. *Suppose $H=H(z)$ is a smooth operator-valued function acting on a separated Hilbert space $\mathfrak{H}$. For $\mathcal{A}_z\in C_0^{\infty}(\Lambda,\mathfrak{H})$, the following asymptotic expression holds.*

$$
H(W)\int_{z\in\Lambda}\mathcal{A}_z\phi_{z,\mathcal{S}_z}^{\varepsilon}\,d\nu_z=\int_{z\in\Lambda}\left[T_0\mathcal{A}_z+(-\mathrm{i}\varepsilon)T_1\mathcal{A}_z+\cdots\right]\phi_{z,\mathcal{S}_z}^{\varepsilon}\,d\nu_z,
$$

where $\{T_j\}$ is a sequence of local differential operators acting on $C_0^{\infty}(\Lambda,\mathfrak{H})$. In particular, the first two operators are

$$
\begin{aligned}
&T_0\mathcal{A}_z=H(z)\mathcal{A}_z,\\
&T_1\mathcal{A}_z=\frac{1}{2}\mathrm{tr}\left[\Pi_z(\mathrm{i}I-J)\nabla^2H(z)\right]\mathcal{A}_z+\mathrm{div}_{\Lambda}\left[\Pi_z(J-\mathrm{i}I)\nabla H(z)\mathcal{A}_z\right].
\end{aligned}
$$

Proof. Recalling the definition of the representation ρ_{ε}, see (2.1), it is direct to verify that

$$
\begin{aligned}
&\rho_{\varepsilon}(\varepsilon w)\rho_{\varepsilon}(-z)\phi^{\varepsilon}\\
&=\exp(\mathrm{i}[w,z])\exp\left[-\varepsilon v^{\dagger}(v+\mathrm{i}u)/2\right]\exp[-(v+\mathrm{i}u)^{\dagger}(x-q)]\rho_{\varepsilon}(-z)\phi^{\varepsilon},
\end{aligned}
$$

which implies

$$
\rho_{\varepsilon}(\varepsilon w)\phi_{z,\mathcal{S}_z}^{\varepsilon}=\exp(\mathrm{i}[w,z])\exp\left[-\varepsilon v^{\dagger}(v+\mathrm{i}u)/2\right]\exp[-(v+\mathrm{i}u)^{\dagger}(x-q)]\phi_{z,\mathcal{S}_z}^{\varepsilon}. \tag{4.6}
$$

Recalling the definition of Weyl's quantization (2.2), we then derive

$$
\begin{aligned}
&H(W)\int_{z\in\Lambda}\mathcal{A}_z\phi_{z,\mathcal{S}_z}^{\varepsilon}\,d\nu_z\\
&=\int_w\int_{z\in\Lambda}\hat{H}(w)\mathcal{A}_z\rho_{\varepsilon}(\varepsilon w)\phi_{z,\mathcal{S}_z}^{\varepsilon}\,d\nu_z dw\\
&=\int_{w=(v;u)}\int_{z=(q;p)\in\Lambda}\hat{H}(w)\exp(\mathrm{i}[w,z])\mathcal{A}_z\exp\left(-\varepsilon v^{\dagger}(v+\mathrm{i}u)/2\right)\\
&\qquad\qquad\times\exp[-(v+\mathrm{i}u)^{\dagger}(x-q)]\phi_{z,\mathcal{S}_z}^{\varepsilon}\,d\nu_z dw,
\end{aligned} \tag{4.7}
$$

where the last line comes from Equation (4.6). By the Taylor expansion of the exponential terms, we have

$$
\exp\left(-\varepsilon v^{\dagger}(v+\mathrm{i}u)/2\right)\exp[-(v+\mathrm{i}u)^{\dagger}(x-q)]
$$

$$\sim 1-\frac{\varepsilon v^\dagger(v+iu)}{2}-(v+\mathrm{i}u)^\dagger(x-q)+\frac{[(v+\mathrm{i}u)^\dagger(x-q)]^2}{2}+\cdots.$$

Applying Lemma 4.2, we can discover the zeroth- and the first-order term in (4.7). In fact, we obtain

$$T_0\mathcal{A}_z=\int_{w=(v;u)}\hat{H}(w)\exp(\mathrm{i}[w,z])\mathcal{A}_z dw=H(z)\mathcal{A}_z,$$

and

$$T_1\mathcal{A}_z=\int_{w=(v;u)}\tilde{T}_1(v;u)\left[\hat{H}(w)\exp(\mathrm{i}[w,z])\mathcal{A}_z\right]dw,$$

where the operator $\tilde{T}_1(v;u)$ is defined as follows

$$\tilde{T}_1(v;u)\mathcal{B}(z)=-\frac{\mathrm{i}v^\dagger(v+\mathrm{i}u)}{2}\mathcal{B}(z)-\mathrm{div}_\Lambda[E_z(v+\mathrm{i}u)\mathcal{B}(z)]+\frac{(v+\mathrm{i}u)^\dagger\mathcal{T}_z(v+\mathrm{i}u)}{2}\mathcal{B}(z),$$

with

$$E_z=\begin{bmatrix}E_{z,1}&\cdots&E_{z,N}\end{bmatrix}=\Pi_z\begin{bmatrix}-\mathrm{i}I\\-I\end{bmatrix},\quad \mathcal{T}_z=(\mathcal{T}_{z,mn}).$$

The formula of $\tilde{T}_1$ can be further simplified by summing the first and the last term, i.e.,

$$\frac{(v+\mathrm{i}u)^\dagger\mathcal{T}_z(v+\mathrm{i}u)}{2}-\frac{iv^\dagger(v+iu)}{2}=\frac{1}{2}\mathrm{tr}\left[\Pi_z(\mathrm{i}I-J)\begin{pmatrix}-uu^\dagger & uv^\dagger\\ vu^\dagger & -vv^\dagger\end{pmatrix}\right].$$

Thus, by applying inverse symplectic Fourier transformation (2.3), we obtain

$$T_1\mathcal{A}_z=\frac{1}{2}\mathrm{tr}\left[\Pi_z(\mathrm{i}I-J)\nabla^2H(z)\right]\mathcal{A}_z+\mathrm{div}_\Lambda\left[\Pi_z(J-\mathrm{i}I)\nabla H(z)\mathcal{A}_z\right], \tag{4.8}$$

which ends the proof. ∎

4.2. Further simplification of T_1 in the scalar case. In the preceding section, we obtain the expression of the transformed E-WKB function under the action of $H(W)$ by doing calculus on the submanifold Λ. If H is a scalar function and Λ is an H-submanifold embedded into the zero level set of H, we can simplify the troublesome term in (4.8) involving divergence on manifold to be a matrix operation. First, we notice that

$$\Pi_z(J-\mathrm{i}I)\nabla H(z)=J\nabla H(z)=\frac{\partial}{\partial t},$$

where $\frac{\partial}{\partial t}$ stands for the t-coordinate vector field induced by the Hamiltonian H. Recall the tangent frame C defined in (4.2), we derive its evolution equation by differentiating the Hamilton system (4.1), i.e.,

$$\dot{C}=J\nabla^2H(z)C. \tag{4.9}$$

Let $C=QP$ be the polar decomposition, then Equation (4.9) is equivalent to

$$\dot{Q}P+Q\dot{P}=J\nabla^2H(z)QP,$$

By right-multiplying P^{-1} and left-multiplying $Q^\dagger$, we derive

$$Q^\dagger \dot{Q} + \dot{P}P^{-1} = Q^\dagger J \nabla^2 H(z) Q.$$

Taking trace of the above equation yields

$$\mathrm{tr}(\dot{P}P^{-1}) = \mathrm{tr}[Q^\dagger J \nabla^2 H(z) Q] = \mathrm{tr}[\Pi_z J \nabla^2 H(z)],$$

which leads to

$$\mathrm{div}_\Lambda \frac{\partial}{\partial t} = \frac{1}{\det P}\frac{\partial}{\partial t}\det P = \mathrm{tr}(\dot{P}P^{-1}) = \mathrm{tr}[\Pi_z J \nabla^2 H(z)]$$

and

$$\mathrm{div}_\Lambda [\Pi_z (J - \mathrm{i}I)\nabla H(z)\mathcal{A}_z] = \mathrm{tr}[\Pi_z J \nabla^2 H(z)]\mathcal{A}_z + \dot{\mathcal{A}}_z.$$

Therefore, we have

$$T_1 \mathcal{A}_z = \frac{1}{2}\mathrm{tr}\left[\Pi_z(\mathrm{i}I + J)\nabla^2 H(z)\right]\mathcal{A}_z + \dot{\mathcal{A}}_z. \tag{4.10}$$

5. E-WKB analysis for vectorial wave equation

In this section, we apply the E-WKB analysis to Equation (2.4) in the vectorial case. In other words, the Hamiltonian $H = H(z)$ is a smooth self-adjoint operator-valued function with compact resolvent, acting on a proper separated Hilbert space $\mathfrak{H}$. In order to seek an approximate solution in the form of (4.3), i.e.,

$$u^\varepsilon = \int_{z\in\Lambda} [\mathcal{A}_z + (-\mathrm{i}\varepsilon)\mathcal{A}_{1,z} + \cdots]\,\phi^\varepsilon_{z,\mathcal{S}_z} d\nu_z, \tag{5.1}$$

there are two main tasks to fulfill. One is to determine the Lagrangian submanifold Λ, and the other is to derive the governing equations of the amplitudes $\mathcal{A}_{k,z}$ and the phase $\mathcal{S}_z$, which are functions defined on Λ. By applying Theorem 4.2, we know that if u^ε given in (5.1) is a first-order asymptotic solution of the Equation (2.4), the following equations must remain valid:

$$H(z)\mathcal{A}_z = 0, \quad \forall z \in \Lambda, \tag{5.2}$$

$$H(z)\mathcal{A}_{1,z} + T_1\mathcal{A}_z = 0, \quad \forall z \in \Lambda. \tag{5.3}$$

From Equation (5.2), there exists an eigenvalue $\lambda(z)$ and its corresponding eigenspace $E(z)$ of $H(z)$ such that Λ is embedded into the zero level set of $\lambda(z)$ and $\mathcal{A}_z \in E(z)$. Furthermore, we assume that the dimension of $E(z)$ is a constant κ. Then we form the Lagrangian submanifold Λ by continuously displacing a connected isotropic submanifold Λ^I_{N-1} which is embedded into the zero level set of $\lambda(z)$ according to the Hamiltonian system (4.1). Moreover, let $\mathcal{S}_0$ be a generating function of the differential 1-form $p^\dagger dq - d(p^\dagger q)/2$ constrained on the isotropic submanifold Λ^{N-1}_I, then the solution $\mathcal{S}_z$ of the following ODE problem

$$\dot{\mathcal{S}}_z + [z, \dot{z}]/2 = 0, \quad \mathcal{S}_z|_{t=0} = \mathcal{S}_0 \in C^\infty(\Lambda^I_{N-1}, \mathbb{R}) \tag{5.4}$$

is also a generating function of that differential 1-form constrained on the Lagrangian submanifold Λ. Now, only the amplitude function $\mathcal{A}_z$ remains to be determined. As in the classical WKB analysis, we introduce the projection $\mathcal{P}(z)$ from $\mathfrak{H}$ to $E(z)$ and derive the following equation independent of $\mathcal{A}_{1,z}$ from Equation (5.3),

$$\mathcal{P}(z)T_1\mathcal{A}_z = 0, \quad \forall z \in \Lambda. \tag{5.5}$$

In the vectorial case, the Equation (5.5) is more complicated to deal with than in the scalar case. In the next section, we first introduce some useful results on the difference between the Hamiltonian $H(z)$ and $\lambda(z)$.

5.1. Some useful results. We introduce a new term $\tilde{H}(z)$ which measures the difference between the Hamiltonian and the scalar one $\lambda(z)$, i.e.,

$$\tilde{H}(z) = H(z) - \lambda(z).$$

Given any smooth function $\mathcal{B}(z)$ defined in a neighborhood of Λ with $\mathcal{B}(z) \in E(z)$, we have

$$\tilde{H}(z)\mathcal{B}(z) = [H(z) - \lambda(z)]\mathcal{B}(z) = 0.$$

By differentiating the above equation with respect to z, we have

$$\nabla \tilde{H}(z)\mathcal{B}(z) + \tilde{H}(z)\nabla\mathcal{B}(z) = 0, \tag{5.6}$$

$$\nabla^2 \tilde{H}(z)\mathcal{B}(z) + \nabla\tilde{H}(z)\nabla^\dagger\mathcal{B}(z) + \nabla\mathcal{B}(z)\nabla^\dagger\tilde{H}(z) + \tilde{H}(z)\nabla^2\mathcal{B}(z) = 0. \tag{5.7}$$

Since

$$\mathcal{P}(z)\tilde{H}(z) = \mathcal{P}(z)[H(z) - \lambda(z)] = 0,$$

applying the projection operator $\mathcal{P}$ onto (5.6) and (5.7) yields

$$\mathcal{P}(z)\nabla\tilde{H}(z)\mathcal{B}(z) = 0, \tag{5.8}$$

and

$$\mathcal{P}(z)\nabla^2\tilde{H}(z)\mathcal{B}(z) + \mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger\mathcal{B}(z) + \left[\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger\mathcal{B}(z)\right]^\dagger = 0. \tag{5.9}$$

5.2. Simplification of the Operator $\mathcal{P}(z)T_1$. Recalling the definition of T_1 in (4.8), we make the following decomposition.

$$\begin{aligned}
T_1\mathcal{B}(z) &= \frac{1}{2}\mathrm{tr}\left[\Pi_z(\mathrm{i}I - J)\nabla^2 H(z)\right]\mathcal{B}(z) + \mathrm{div}_\Lambda\left[\Pi_z(J - \mathrm{i}I)\nabla H(z)\mathcal{B}(z)\right] \\
&= \frac{1}{2}\mathrm{tr}\left[\Pi_z(\mathrm{i}I - J)\nabla^2 \lambda(z)\right]\mathcal{B}(z) + \mathrm{div}_\Lambda\left[\Pi_z(J - \mathrm{i}I)\nabla \lambda(z)\mathcal{B}(z)\right] \\
&\quad + \frac{1}{2}\mathrm{tr}\left[\Pi_z(\mathrm{i}I - J)\nabla^2 \tilde{H}(z)\right]\mathcal{B}(z) + \mathrm{div}_\Lambda\left[\Pi_z(J - \mathrm{i}I)\nabla \tilde{H}(z)\mathcal{B}(z)\right] \\
&\equiv \square_1 + \square_2,
\end{aligned}$$

where $\square_1$ refers to the second line, and $\square_2$ refers to the third line.

We notice that $\square_1$ is exactly the expression of T_1 in the scalar case, which can be simplified as (4.10), i.e.,

$$\square_1 = \frac{1}{2}\mathrm{tr}\left[\Pi_z(\mathrm{i}I + J)\nabla^2\lambda(z)\right]\mathcal{B}(z) + \dot{\mathcal{B}}(z), \quad z \in \Lambda. \tag{5.10}$$

To simplify $\square_2$, we perform a direct computation and obtain

$$\begin{aligned}
&\mathrm{div}_\Lambda\left[\Pi_z(J - \mathrm{i}I)\nabla\tilde{H}(z)\mathcal{B}(z)\right] \\
&= \mathrm{tr}\left[\Pi_z(J - \mathrm{i}I)\nabla^\dagger(\nabla\tilde{H}(z)\mathcal{B}(z))\right] + \mathrm{div}_\Lambda\left[\Pi_z(J - \mathrm{i}I)\right]\nabla\tilde{H}(z)\mathcal{B}(z).
\end{aligned} \tag{5.11}$$

Applying the projection operator $\mathcal{P}$ onto Equation (5.11) and recalling (5.8), we know that for all $z \in \Lambda$, it holds that

$$\mathcal{P}(z)\mathrm{div}_\Lambda\left[\Pi_z(J - \mathrm{i}I)\nabla\tilde{H}(z)\mathcal{B}(z)\right] = \mathcal{P}(z)\mathrm{tr}\left[\Pi_z(J - \mathrm{i}I)\nabla^\dagger(\nabla\tilde{H}(z)\mathcal{B}(z))\right].$$

By applying (5.9) and the above result, we arrive at

$$\begin{aligned}
\mathcal{P}(z)\Box_2 =& \mathcal{P}(z)\frac{1}{2}\mathrm{tr}\left[\Pi_z(\mathrm{i}I-J)\nabla^2\tilde{H}(z)\right]\mathcal{B}(z)-\mathcal{P}(z)\mathrm{tr}\left[\Pi_z(\mathrm{i}I-J)\nabla^\dagger(\nabla\tilde{H}(z)\mathcal{B}(z))\right]\\
=&\frac{1}{2}\mathrm{tr}\left[\Pi_z(\mathrm{i}I-J)\left(-\mathcal{P}(z)\nabla^2\tilde{H}(z)\mathcal{B}(z)-2\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger\mathcal{B}(z)\right)\right]\\
=&\frac{1}{2}\mathrm{tr}\left[\Pi_z(\mathrm{i}I-J)\left(\left[\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger\mathcal{B}(z)\right]^\dagger-\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger\mathcal{B}(z)\right)\right]\\
=&\frac{1}{2}\mathrm{tr}\left[\Pi_z\left(J\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger\mathcal{B}(z)+\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger\mathcal{B}(z)J\right)\right]\\
=&\frac{1}{2}\mathrm{tr}\left[\Pi_z\{J,\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger\mathcal{B}(z)\}\right].
\end{aligned}$$

In the above, $\{A,B\}=AB+BA$ denotes the anti-commutator. For any $E(z)$-valued smooth function $\mathcal{B}(z)$ defined on the phase space $\mathbb{R}^{2N}$, let us introduce the following matrix-$E(z)$-valued operator L as

$$L\mathcal{B}(z)=\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger\mathcal{B}(z). \tag{5.12}$$

With this operator introduced, we then have

$$\mathcal{P}(z)\Box_2=\frac{1}{2}\mathrm{tr}\left[\Pi_z\{J,L\}\right]\mathcal{B}(z).$$

Combining the above with Equation (5.10) yields

$$\mathcal{P}(z)T_1\mathcal{B}(z)=\mathcal{P}(z)\dot{\mathcal{B}}(z)+\frac{1}{2}\mathrm{tr}\left[\Pi_z(\mathrm{i}I+J)\nabla^2\lambda(z)\right]\mathcal{B}(z)+\frac{1}{2}\mathrm{tr}\left(\Pi_z\{J,L\}\right)\mathcal{B}(z). \tag{5.13}$$

5.3. Derivation of amplitude equation. In order to express $\mathcal{P}(z)T_1\mathcal{A}_z$ in the form of (5.13), we first prove that L is well-defined as a pointwise map from $E(z)$ to $E(z)^{2N\times 2N}$, i.e., a matrix with entries belonging to $E(z)$. To be precise, suppose that $\mathcal{A}_z\in E(z)$ with a representation $\mathcal{A}_z=\sigma_z^\beta b_\beta(z)$, where $\{b_\beta(z)\}_{\beta=1}^\kappa$ forms a smooth basis for $E(z)$. Here and hereafter, the Einstein summation convention is adopted. Let $\sigma^\beta(z)$ be any smooth extension of σ_z^β in a neighborhood of z. We have

$$\begin{aligned}
L(\sigma^\beta(z)b_\beta(z))&=\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger(\sigma^\beta(z)b_\beta(z))\\
&=\sigma_z^\beta\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger b_\beta(z),
\end{aligned}$$

which is independent of the choice of extension.

Next we show that the action of L on $E(z)$ is independent of the choice of basis of $E(z)$. Given another smooth set of basis functions $\{\tilde{b}_\beta(z)\}_{\beta=1}^\kappa$ of $E(z)$, we know that there exists a smooth family of invertible matrices $(c_\beta^\alpha(z))$ such that $\tilde{b}_\beta(z)=c_\beta^\gamma(z)b_\gamma(z)$. Suppose that $\mathcal{A}_z=\tilde{\sigma}_z^\beta\tilde{b}_\beta(z)$ is a new representation, and $\tilde{\mathcal{B}}(z)$ is any extension of $\mathcal{A}_z$ under this new set of basis functions, we have

$$\begin{aligned}
L\tilde{\mathcal{B}}(z)&=\tilde{\sigma}_z^\beta\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger\tilde{b}_\beta(z)\\
&=\tilde{\sigma}_z^\beta\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger\left[c_\beta^\gamma(z)b_\gamma(z)\right]\\
&=\tilde{\sigma}_z^\beta c_\beta^\gamma(z)\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger b_\gamma(z)\\
&=\sigma_z^\gamma\mathcal{P}(z)\nabla\tilde{H}(z)\nabla^\dagger b_\gamma(z)=L\mathcal{B}(z).
\end{aligned}$$

Thus L is well-defined as a pointwise map from $E(z)$ to $E(z)^{2N\times 2N}$. As a result, the Equation (5.13) holds for the leading order amplitude function $\mathcal{A}_z \in E(z)$,

$$\mathcal{P}(z)\dot{\mathcal{A}}_z + \frac{1}{2}\mathrm{tr}\left[\Pi_z(\mathrm{i}I+J)\nabla^2\lambda(z)\right]\mathcal{A}_z + \frac{1}{2}\mathrm{tr}\left(\Pi_z\{J,L\}\right)\mathcal{A}_z = 0. \tag{5.14}$$

Using $\langle \cdot\,,\,\cdot\rangle$ to denote the inner product of Hilbert Space $\mathfrak{H}$ and setting

$$\begin{aligned}
&M_{\alpha,\beta}(z) = \langle b_\alpha(z), b_\beta(z)\rangle,\\
&\varpi_z = \mathrm{tr}\left[\Pi_z(\mathrm{i}I+J)\nabla^2\lambda(z)\right],\\
&W_{\alpha,\beta}(z) = \langle b_\alpha(z), \dot{b}_\beta(z)\rangle = \langle b_\alpha(z), \nabla b_\beta(z) J\nabla\lambda(z)\rangle,\\
&L_{\alpha,\beta}(z) = \langle b_\alpha(z), \nabla\tilde{H}(z)\nabla^\dagger b_\beta(z)\rangle,
\end{aligned}$$

the amplitude Equation (5.14) is equivalent to the following ODE system

$$M_{\alpha,\beta}\dot{\sigma}_z^\beta + W_{\alpha,\beta}\sigma_z^\beta + \frac{1}{2}\varpi_z M_{\alpha,\beta}\sigma_z^\beta + \frac{1}{2}\mathrm{tr}\left[\Pi_z\{J, L_{\alpha,\beta}\}\right]\sigma_z^\beta = 0, \tag{5.15}$$

where $\Pi_z = QQ^\dagger$, $Q = C(C^\dagger C)^{-\frac{1}{2}}$. Omitting the higher order terms in (5.1), we derive a first-order asymptotic approximation of the solution u^ε through the following integral on the Lagrangian submanifold Λ, i.e.,

$$u^\varepsilon_{E-WKB} = \int_\Lambda \mathcal{A}_z \phi^\varepsilon_{z,\mathcal{S}_z}\, d\nu_z. \tag{5.16}$$

6. Well-prepared data for time harmonic problem

In this section, we discuss the details on numerical computation of the time harmonic problem (2.4) with well-prepared WKB-form incident value given on an incident submanifold Λ_I^{N-1}. Since for all $z \in \mathbb{R}^{2N}$, $H(z)$ is a self-adjoint operator with compact resolvent. This means that $H(z)$ has countable eigenvalues $\{\lambda_\alpha(z)\}$ and their associated eigenspace sets are $\{E_\alpha(z)\}$. But not all the eigenspaces are suitable to give an incident value on and not all the WKB functions can be chosen as an incident value. They must satisfy some necessary conditions.

6.1. Compatible conditions.

Suppose $\lambda(z)$ is a specific eigenvalue such that the corresponding zero level set forms a submanifold of dimension $2N-1$ in the phase space. The Cauchy data for the vectorial wave Equation (2.4) are prescribed on a connected submanifold Γ of dimension $N-1$ in position space as follows:

$$u_I^\varepsilon(x) = A_I(x)\exp\left[\mathrm{i}S_I(x)/\varepsilon\right],\ x\in\Gamma, \tag{6.1}$$

where $A_I(x) \in C_0^\infty(\Gamma, \mathfrak{H})$ and $S_I(x) \in C^\infty(\Gamma, \mathbb{R})$. Additional requirements should be imposed on Γ, $S_I(x)$, $A_I(x)$ and other quantities. We will clarify this point in the sequel.

First we intend to seek a local WKB solution associated with the λ-submanifold,

$$u^\varepsilon(x) = \left[A(x) + \mathcal{O}(\varepsilon)\right]\exp\left[\mathrm{i}S(x)/\varepsilon\right].$$

As revealed, the phase function $S(x)$ should satisfy the Hamilton-Jacobi Equation (3.4). Confined to Γ, we have

$$\nabla S(x) = \nabla_\Gamma S_I(x) + \nabla_\Gamma^\perp S(x),\ x\in\Gamma.$$

Substituting the above into (3.4) yields

$$\lambda(x, \nabla_\Gamma S_I(x) + \nabla_\Gamma^\perp S(x)) = 0,\ x\in\Gamma. \tag{6.2}$$

Since Γ has a codimension of 1 in $\mathbb{R}^N$ and $\nabla_\Gamma S_I(x)$ is determined by $S_I(x)$, the above equation is actually a (generally) nonlinear algebraic equation with respect to $\nabla_\Gamma^\perp S(x)$. We assume that Γ and S_I are specified in a way such that there exists at least one smooth family of solutions. Note that such kind of family might not be unique, and different families typically correspond to different traveling wave modes.

By specifying the traveling wave mode, we derive an initial isotropic submanifold Λ_I^{N-1} in the phase space

$$\Lambda_I^{N-1} = \{(q;p) \in \mathbb{R}^{2N} \mid p = \nabla_\Gamma S_I(q) + \nabla_\Gamma^\perp S(q),\ q \in \Gamma\}.$$

Obviously, Λ_I^{N-1} is a graph submanifold. To ensure the existence of a local WKB solution, we need to assume that a local continuous displacement of Λ_I^{N-1} by the λ-Hamiltonian flow forms a local graph Lagrangian submanifold. A sufficient condition for this to be valid is the transversality of the velocity field to Γ. This means that for all $(q;p) \in \Lambda_I^{N-1}$, the velocity $\nabla_p \lambda(q,p)$ has a nonvanishing normal component. Note that $A_I(x)$ should lie in the eigenspace $E(z)$, so the third compatible condition is

$$A_I(q_I) \in E(q_I;p_I),\ \forall (q_I;p_I) \in \Lambda_I^{N-1}.$$

6.2. Initial phase and amplitude for E-WKB solution. To determine the first-order E-WKB asymptotic solution (5.16), we need to specify the initial phase and amplitude function on the initial isotropic submanifold Λ_I^{N-1}. By Theorem 4.1, we have

$$\mathcal{S}_z = S_I(q) - p^\dagger q/2,\ \forall z = (q;p) \in \Lambda_I^{N-1}, \tag{6.3}$$

and

$$\mathcal{A}_z = \det{}^{-\frac{1}{2}} \left(I - \mathrm{i}\frac{\partial p}{\partial q} \right) A_I(q),\ \forall z = (q;p) \in \Lambda_I^{N-1}. \tag{6.4}$$

Therefore, to determine $\mathcal{A}_z$ on the initial submanifold, we need to compute $\dfrac{\partial p}{\partial q}$ for all $z \in \Lambda_I^{N-1}$. Let y be a coordinate of Γ, which is also a coordinate of the graph manifold Λ_I^{N-1}. Then (y,t) forms a coordinate for the Lagrangian submanifold Λ. As defined in (4.2), we have

$$C = \frac{\partial(q;p)}{\partial(y;t)} = \begin{bmatrix} U \\ V \end{bmatrix}, \quad U,V \in \mathbb{R}^{N\times N}.$$

Thanks to the Hamiltonian system (4.1), it holds that

$$\begin{aligned} U &= \frac{\partial q}{\partial(y;t)} = \begin{bmatrix} \dfrac{\partial q}{\partial y} & \nabla_p \lambda(q;p) \end{bmatrix}, \\ V &= \frac{\partial p}{\partial(y;t)} = \begin{bmatrix} \dfrac{\partial p}{\partial y} & -\nabla_q \lambda(q;p) \end{bmatrix}. \end{aligned}$$

This leads to

$$\frac{\partial p}{\partial q} = \frac{\partial p}{\partial(y;t)} \frac{\partial(y;t)}{\partial q} = VU^{-1},\ z \in \Lambda_I^{N-1}. \tag{6.5}$$

6.3. First-order E-WKB approximation. After determining the initial isotropic submanifold Λ_I^{N-1} and the initial data functions $\mathcal{A}_z$, $\mathcal{S}_z$ and $C|_{\Lambda_I^{N-1}}$, we will derive the following E-WKB asymptotic solution in the global (y,t) coordinates

$$u^{\varepsilon}_{E-WKB} = \int_{(y,t)\in\Gamma\times\mathbb{R}} \mathcal{A}_z \phi^{\varepsilon}_{z,\mathcal{S}_z} \det(C^{\dagger}C)^{\frac{1}{2}} dydt. \tag{6.6}$$

Until now, we have obtained evolution equations for rays, moving frames, phase function and amplitude functions, see (4.1), (4.9), (5.4), (5.15) respectively. These equations consist of the following ODE system from which we can compute the E-WKB approximate solution.

$$\begin{aligned}
&\dot{z} = J\nabla\lambda(z),\\
&\dot{C} = J\nabla^2\lambda(z)C,\\
&\dot{\mathcal{S}}_z + [z,\dot{z}]/2 = 0,\\
&M_{\alpha,\beta}\dot{\sigma}^{\beta}_z + W_{\alpha,\beta}\sigma^{\beta}_z + \frac{1}{2}\varpi_z M_{\alpha,\beta}\sigma^{\beta}_z + \frac{1}{2}\mathrm{tr}(\Pi_z\{J,L_{\alpha,\beta}\})\sigma^{\beta}_z = 0.
\end{aligned} \tag{6.7}$$

The initial condition is specified on Λ_I^{N-1} as

$$\begin{aligned}
&z|_{t=0} = (q_I,p_I) \in \Lambda_I^{N-1},\\
&C|_{t=0} = C|_{\Lambda_I^{N-1}},\\
&\mathcal{S}_z|_{t=0} = \mathcal{S}_z|_{\Lambda_I^{N-1}},\\
&\sigma^{\alpha}_z|_{t=0} = \sigma^{\alpha}_z|_{\Lambda_I^{N-1}}.
\end{aligned}$$

7. Numerical tests

In this section, we apply the E-WKB analysis to vectorial Schrödinger equation and 2-D Helmholtz equation to check the effectiveness of our method. There are three main steps in the E-WKB analysis. First, we formulate the problem in the canonical form (2.4) and derive the eigen-pair $\lambda(z)$ and $E(z)$ for the Hamiltonian $H(z)$. Second, we choose incident data which are of WKB form defined on an $N-1$ dimensional manifold Γ in the position space. The last part is to solve the ODE system (6.7) and compute the integral (6.6) on the Lagrangian submanifold. In both the examples, a first-order convergence rate of the asymptotic error is demonstrated, even beyond the caustic points.

7.1. Vectorial Schrödinger equation. In this subsection, we consider the vectorial Schrödinger equation

$$-i\varepsilon\frac{\partial}{\partial t}\mathbf{u} - \frac{\varepsilon^2}{2}\frac{\partial^2}{\partial x^2}\mathbf{u} + V(x)\mathbf{u} = 0, \tag{7.1}$$

where the potential is prescribed as

$$V(x) = \frac{x^2}{2} + \begin{pmatrix} \cos 2x & -\sin 2x \\ -\sin 2x & -\cos 2x \end{pmatrix}.$$

The initial data are specified in the WKB form

$$u_I(x) = \exp(-16(x-2)^2)\exp\left(\frac{ix^2}{6\varepsilon}\right)\begin{pmatrix}\cos x\\ -\sin x\end{pmatrix}. \tag{7.2}$$

In order to apply the theory developed in this paper, the time evolution problem is transformed into a time harmonic one by regarding t as a "position" variable. By introducing the dual variables of x and t as p and η, we can rewrite the Hamiltonian

$$-i\varepsilon\frac{\partial}{\partial t}-\frac{\varepsilon^2}{2}\frac{\partial^2}{\partial x^2}+\frac{x^2}{2}+\begin{pmatrix}\cos 2x & -\sin 2x\\ -\sin 2x & -\cos 2x\end{pmatrix}$$

as Weyl quantization of the following vector valued function defined in phase space

$$H(q,t,p,\eta)=\eta+\frac{p^2+q^2}{2}+\begin{pmatrix}\cos 2q & -\sin 2q\\ -\sin 2q & -\cos 2q\end{pmatrix}.$$

The eigen-pairs of H are

$$\lambda_+=\eta+\frac{p^2+q^2}{2}+1,\quad b_+=\begin{pmatrix}\cos q\\ -\sin q\end{pmatrix},$$
$$\lambda_-=\eta+\frac{p^2+q^2}{2}-1,\quad b_-=\begin{pmatrix}\sin q\\ \cos q\end{pmatrix},$$

which represent two separate energy surfaces. Since the initial vector (7.2) is parallel to b_+, the solution is constrained on the top energy surface, i.e., λ_+, during evolution. Then rays are traced by the Hamiltonian system associated with λ_+:

$$\dot{z}=J\nabla\lambda_+(z).$$

More explicitly, if we introduce the hidden temporal variable as τ, we obtain

$$\frac{dq}{d\tau}=p,\quad t=\tau,\quad \frac{dp}{d\tau}=-q,\quad \frac{d\eta}{d\tau}=0.$$

In particular, for initial point $(q_0,0,p_0,\eta_0)$, the exact solution of q can be expressed as

$$q(\tau)=q_0\cos(\tau)+p_0\sin(\tau). \tag{7.3}$$

Next step is to determine the incident submanifold Λ_I in phase space, which should be of dimension 1. We truncate the support set of the incident data (7.2) as $\Gamma=[1,3]$. Then we obtain the parameterization of the incident submanifold Λ_I

$$\Lambda_I=\left\{(q,t,p,\eta)|q\in\Gamma,\ t=0,\ p=q/3,\ \eta=-\frac{5q^2}{9}-1\right\},$$

where p is determined by phase at $t=0$, i.e., $S_I(x)=x^2/6$ and η is obtained by solving local WKB solution from the Hamilton-Jacobi equation

$$\lambda_+(q,t,\nabla S_I,\eta)=\eta+\frac{\nabla^2 S_I+q^2}{2}+1=0.$$

It is remarkable that for $p_0=q_0/3$, and $\tau=\pi-\tan^{-1}3\approx 1.89$, we have $q(\tau)=0$, which means that all rays concentrate over $q=0$ at τ. The ODE system is formulated as follows. For rays and frames, we have

$$\dot{z}=J\nabla\lambda_+(z),$$
$$\dot{C}=J\nabla^2\lambda_+(z)C,$$

with initial data specified as

$$z_I=\begin{pmatrix} q\\ 0\\ q/3\\ -5q^2/9-1\end{pmatrix},\quad C_I=\begin{pmatrix}\dfrac{\partial z_I}{\partial q} & \dfrac{\partial z_I}{\partial \tau}\end{pmatrix}=\begin{pmatrix}1 & q/3\\ 0 & 1\\ 1/3 & -q\\ -10q/9 & 0\end{pmatrix}=\begin{pmatrix}U\\ V\end{pmatrix}. \tag{7.4}$$

For phase and amplitude, they satisfy the following governing equations

$$\dot{\mathcal{S}}_z+[z,\dot z]/2=0, \tag{7.5}$$

$$\dot\sigma_z+\langle b_+,\nabla^\dagger b_+J\nabla\lambda_+\rangle\sigma_z+\frac{1}{2}\mathrm{tr}\left[\Pi_z(iI+J)\nabla^2\lambda_+\right]\sigma_z+\frac{1}{2}\mathrm{tr}\left(\Pi_z\{J,L\}\right)\sigma_z=0, \tag{7.6}$$

where

$$\begin{aligned}&\nabla^\dagger b_+=\left(\partial_q b_+\ \partial_t b_+\ \partial_p b_+\ \partial_\eta b_+\right),\\ &\Pi_z=C(C^\dagger C)^{-1}C^\dagger,\\ &L_{ij}=\langle b_+,\partial_i(H-\lambda_+)\partial_j b_+\rangle,\quad i,j\in\{1,2,3,4\},\end{aligned}$$

with $\partial_1=\partial_q$, $\partial_2=\partial_t$, $\partial_3=\partial_p$, $\partial_4=\partial_\eta$.

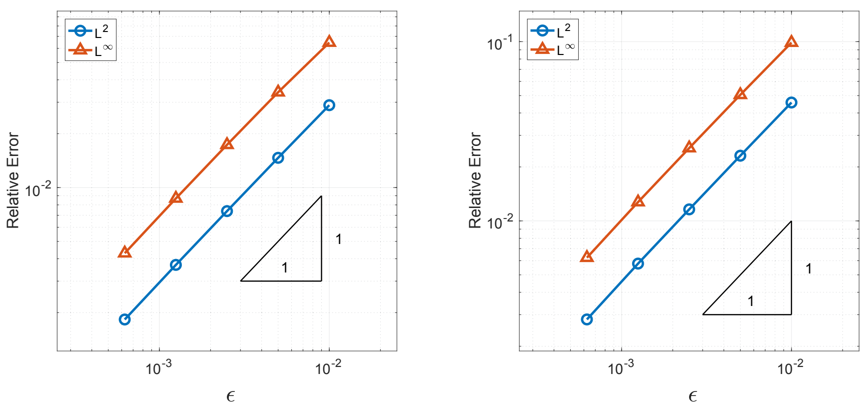

FIG. 7.1. *Relative error* $\dfrac{\|\hat u-u^\varepsilon\|.}{\|\hat u\|.}$ *between reference solution* $\hat u$ *and E-WKB solution* u^ε. *They are measured in* L^2 *and* L^∞ *at* $t=1$ *(left) and* $t=3$ *(right). The numerical solutions are computed with* $\varepsilon=10^{-2}/2^k$ *with* $k=0,1,\cdots,4$.

By (6.3)-(6.4), the initial data for phase and amplitude are specified as

$$\begin{aligned}&\mathcal{S}_z=S_I(q)-\frac{p^\dagger q}{2}=0,\\ &\sigma_z=\exp(-16(q-2)^2)\det{}^{-\frac{1}{2}}(I-iVU^{-1}),\quad z\in\Lambda_I.\end{aligned}$$

In the numerical implementation of E-WKB method, Γ is discretized equidistantly into 200 nodes, and the ODE system (7.4)-(7.6) is solved by the classical Runge-Kutta method, with $\Delta t=2\times10^{-3}$. The relative error is computed in domain $[-5,5]$ between the E-WKB approximate solution and the reference solution which is computed by operator splitting spectral method. Both L^2 and L^∞ norms are chosen to demonstrate the error convergence. As is demonstrated in Figure. 7.1, at $t=1$ and $t=3$, the E-WKB approximate solution converges at an order $\mathcal{O}(\varepsilon)$. Caustics have no effect on the performance of our algorithm.

7.2. Helmholtz equation. In this numerical experiment, we consider the 2-D Helmholtz equation,

$$\Delta P(x)+\omega^2 P(x)=0, \quad x\in\mathbb{R}^2, \tag{7.7}$$

with prescribed incident pressure

$$P_{inc}(x)=\frac{H_0^{(2)}(\omega r)}{H_0^{(2)}(\omega)}, \quad r=|x|. \tag{7.8}$$

The total pressure field has an analytical expression

$$P(x)=\frac{2J_0(\omega r)}{H_0^{(2)}(\omega)}, \quad r=|x|,$$

where $H_0^{(2)}$ stands for the second kind Hankel function of order 0, J_0 is the first kind Bessel function of order 0.

Although (7.7) is a scalar equation, and can be solved by the scalar-type E-WKB method introduced in [19], we can transform (7.7) into the following vectorial form

$$\begin{aligned} -P-i\varepsilon\nabla\cdot\mathbf{U}=0,\\ -\mathbf{U}-i\varepsilon\nabla P=0, \end{aligned}$$

where $\varepsilon=\omega^{-1}$. The above system is equivalent to the general vectorial wave equation (2.4) with

$$u^\varepsilon=(P;\mathbf{U}), \quad H=\begin{bmatrix}-1 & p^\dagger\\ p & -I\end{bmatrix}.$$

In this experiment, we are interested in the following eigenpair of H,

$$\lambda(q,p)=|p|-1, \quad b=\left[|p| \; p_1 \; p_2\right]^\dagger.$$

Therefore, we assume that the incident wave propagates inward and is proportional to b. Moreover, the incident surface is assumed to be $\Gamma=\{x||x|=r_I\}$ and the Lagrangian submanifold lies in $\lambda(q,p)=0$. As a result, we obtain the formulation of the 1-D initial submanifold,

$$\Lambda_I=\{(q_1,q_2,p_1,p_2)|q_1=r_I\cos\theta,\ q_2=r_I\sin\theta,\ p_1=-\cos\theta,\ p_2=-\sin\theta,\ \theta=[0,2\pi]\}.$$

Thus, we derive the parameterization of the incident surface as well as the representation of the tangent space,

$$z=\begin{bmatrix} r_I\cos\theta\\ r_I\sin\theta\\ -\cos\theta\\ -\sin\theta\end{bmatrix}, \quad C=\begin{bmatrix}\frac{\partial z}{\partial\theta} & \frac{\partial z}{\partial t}\end{bmatrix}=\begin{bmatrix} -r_I\sin\theta & -\cos\theta\\ r_I\cos\theta & -\sin\theta\\ \sin\theta & 0\\ -\cos\theta & 0\end{bmatrix}=\begin{pmatrix}U\\ V\end{pmatrix}.$$

Since $p=(-\cos\theta,-\sin\theta)$, we choose $S_I(x)=-|x|$ so that $p=\nabla S_I(q)$. In order to rewrite the incident pressure (7.8) into the WKB form, we solve for the amplitude from the following vectorial equation with the help of the assumption that the incident wave is proportional to b,

$$\begin{pmatrix} P_{inc}(x) \\ \mathbf{U} \end{pmatrix} = A_I(x)\exp\left(\frac{iS_I(x)}{\varepsilon}\right), \quad x\in\Gamma.$$

Note that the first entry of b is $|p|=1$, as is required by the Hamilton-Jacobi equation $\lambda(x,\nabla S_I(x))=0$. Then, we obtain

$$A_I(x)=\frac{H_0^{(2)}(\omega r)}{H_0^{(2)}(\omega)}\exp\left(\frac{-iS_I(x)}{\varepsilon}\right)b.$$

By (6.3)-(6.4), we obtain the initial values of phase and amplitude on Λ_I:

$$\begin{aligned} \mathcal{S}_z &= S_I(q)-p^\dagger q/2=-\frac{r_I}{2}, \\ \sigma_z &= \frac{H_0^{(2)}(\omega r_I)}{H_0^{(2)}(\omega)}\exp\left(\frac{-\mathrm{i}S_I(q)}{\varepsilon}\right)\det{}^{-\frac{1}{2}}(I-iVU^{-1}), \quad z\in\Lambda_I. \end{aligned} \tag{7.9}$$

The final two steps of the E-WKB method are to solve the ODE system (6.7) with initial data (7.9) and compute the integral (6.6) on the Lagrangian submanifold.

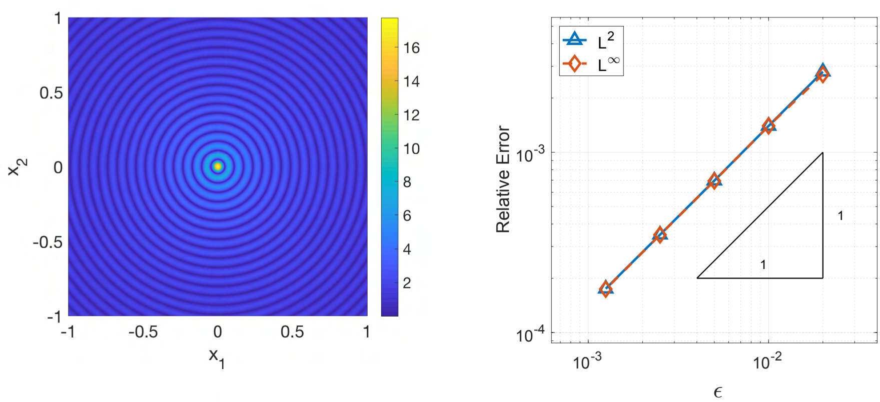

FIG. 7.2. *Left: Pressure field with $\omega=50$, $r_I=2$. Right: Relative error $\frac{||\hat{u}-u^\varepsilon||.}{||\hat{u}||.}$ between the exact solution $\hat{u}$ and the approximate one u^ε. The norms are chosen as L^2 and L^∞ respectively.*

The left of Figure 7.2 shows the numerical solution for pressure field. In this case, all rays gather at the origin, which results in greater pressure there. In the right picture of Figure 7.2, we demonstrate a first-order asymptotic convergence rate of the relative error between the approximate solution and the exact one when measured in L^2 and L^∞ norms.

8. Conclusion

In this paper, we perform the E-WKB analysis to linear vectorial wave equations in the high-frequency regime. The new procedure based on the E-WKB form is parallel to the classical WKB analysis, but remains valid even in the case of the caustic problem. Compared to the local WKB analysis developed in [19], first-order approximate solution is obtained in a more comprehensive way in this paper. It is hoped that high order approximations can be derived via the E-WKB analysis.

Acknowledgements. CZ's work was supported by Natural Science Foundation of Xinjiang Autonomous Region under No. 2019D01C026.

REFERENCES

[1] J.B. Keller, *Corrected Bohr-Sommerfeld quantum conditions for non-separable systems*, Ann. Phys., 4(2):180–188, 1958. 1

[2] V.P. Maslov and M.V. Fedoryuk, *Semi-Classical Approximation in Quantum Mechanics*, Dordrecht Reidel Pub. Co., 1981. 1

[3] V.M. Babič and V.S. Buldyrev, *Short-Wavelength Diffraction Theory: Asymptotic Methods*, Springer Series on Wave Phenomena, Springer-Verlag, 4, 1991. 1

[4] L.V. Hörmander, *On the existence and the regularity of solutions of linear pseudo-differential equations*, Uspekhi Mat. Nauk, 28(6):109–164, 1973. 1

[5] J. Ralston, *Gaussian beams and the propagation of singularities*, in W. Littman (ed.), Studies in Partial Differential Equations, MAA Stud. Math., Math. Assoc. America, Washington DC, 23:206–248, 1983. 1

[6] S. Jin, H. Wu, and X. Yang, *Gaussian beam methods for the Schrödinger equation in the semi-classical regime: Lagrangian and Eulerian formulations*, Commun. Math. Sci., 6(4):995–1020, 2008. 1

[7] S. Jin, H. Wu, and X. Yang, *A numerical study of the Gaussian beam methods for Schrödinger-Poisson equations*, J. Comput. Math., 28(2):261–272, 2010. 1

[8] N.M. Tanushev, *Superpositions and higher order Gaussian beams*, Commun. Math. Sci., 6(2):449–475, 2008. 1

[9] K. Kay, *The Herman-Kluk approximation: derivation and semiclassical corrections*, Chem. Phys., 322(1-2):3–12, 2006. 1

[10] S. Jin, H. Wu, and X. Yang, *Semi-Eulerian and high order Gaussian beam methods for the Schrödinger equation in the semiclassical regime*, Comm. Comput. Phys., 9(3):668–687, 2011. 1

[11] H. Liu and J. Ralston, *Recovery of high frequency wave fields for the acoustic wave equation*, Multiscale Model. Simul., 8(2):428–444, 2009. 1

[12] H. Liu and J. Ralston, *Recovery of high frequency wave fields from phase space-based measurements*, Multiscale Model. Simul., 8(2):622–644, 2010. 1

[13] H. Liu, O. Runborg, and N.M. Tanushev, *Error estimates for Gaussian beam superpositions*, Math. Comp., 82(282):919–952, 2013. 1

[14] M. Motamed and O. Runborg, *Taylor expansion and discretization errors in Gaussian beam superposition*, Wave Motion, 47(7):421–439, 2010. 1

[15] C. Zheng, *Optimal error estimates for first-order Gaussian beam approximations to the Schrödinger equation*, SIAM J. Numer. Anal., 52(6):2905–2930, 2014. 1

[16] S. Bougacha, J.L. Akian, and R. Alexandre, *Gaussian beams summation for the wave equation in a convex domain*, Commun. Math. Sci., 7(4):973–1008, 2009. 1

[17] C. Zheng, *Gaussian beam approach for the boundary value problem of high frequency Helmholtz equation*, Commun. Math. Sci., 8(4):1041–1066, 2010. 1

[18] S. Jin, P.A. Markowich, and C. Sparber, *Mathematical and computational methods for semiclassical Schrödinger equations*, Acta Numer., 20:121–209, 2011. 1

[19] C. Zheng, *Global geometrical optics method*, Commun. Math. Sci., 11(1):105–140, 2013. 1, 4, 7.2, 8

[20] J. Hu, X. Ma, and C. Zheng, *Global geometrical optics method for vector-valued Schrödinger problems*, Front. Math. China, 13(3):579–606, 2018. 1

[21] G.B. Folland, *Harmonic Analysis in Phase Space*, Princeton University Press, 1989. 2.1