

# CONVERGENCE OF FROZEN GAUSSIAN APPROXIMATION FOR HIGH FREQUENCY WAVE PROPAGATION

JIANFENG LU AND XU YANG

ABSTRACT. The frozen Gaussian approximation provides a highly efficient computational method for high frequency wave propagation. The derivation of the method is based on asymptotic analysis. In this paper, for general linear strictly hyperbolic system, we establish the rigorous convergence result for frozen Gaussian approximation. As a byproduct, higher order frozen Gaussian approximation is developed.

## 1. INTRODUCTION

This paper is devoted to the proof of convergence of the frozen Gaussian approximation, introduced in [11, 12], for high frequency wave propagation. Numerical computation of high frequency wave propagation is an important problem concerned in many areas, such as seismic imaging, electromagnetic radiation and scattering, and so on. The problem is challenging for direct numerical discretization because the mesh size has to be chosen comparable to the wavelength or even smaller in order to get accurate solution, however the domain size is usually large so that the computational cost is formidably expensive. To look for efficient computation, the development of asymptotics-based algorithms has received a great amount of attention in recent years.

The investigations have been focused on two methods: geometric optics and Gaussian beam method. The computational methods based on geometric optics (see the review articles [3, 19], and references therein) solve eikonal and transport equations instead of original hyperbolic system. This makes the choice of mesh size frequency-independent, and hence the methods are quite efficient. However, eikonal equation can develop singularities that makes the asymptotic approximation break down at caustics. To overcome this problem, Popov introduced Gaussian beam method in [15], which constructs solution near geometric rays using Taylor expansion. Ralston [17] showed that the method gives a valid approximation at caustics. One shortcoming of Gaussian beam method is however, since it is based on Taylor expansion, the constructed beam solution has to stay near geometric rays to maintain accuracy. Therefore the method loses accuracy when the solution

spreads [12, 14, 16]. The problem is one of the major concerns in application of Gaussian beam methods in areas like seismic imaging; see for example [2, 5].

The frozen Gaussian approximation was proposed in our previous works [11, 12] to overcome the problems of the aforementioned methods: Geometric optics breaks down around caustics; Gaussian beam method loses accuracy when beam spreads. The frozen Gaussian approximation is based on asymptotic analysis on phase plane, motivated by the Herman-Kluk propagator developed in chemistry literature [4, 6, 7]. It provides a highly efficient computational tool for computing high frequent solution to linear hyperbolic system.

Our previous work [11, 12] developed numerical algorithms for frozen Gaussian approximation in both Lagrangian and Eulerian framework. Numerical examples indicate the efficiency and accuracy of the method. In the current work, we prove the convergence of frozen Gaussian approximation. Denote the propagator of the first order strictly hyperbolic system as  $\mathcal{P}_t$ , and the propagator of the  $K$ th-order frozen Gaussian approximation as  $P_{t,K}^\varepsilon$ . The main result of this work is the following theorem.

**Theorem.** *Let  $\{u_0^\varepsilon\}_{\varepsilon>0}$  be a family of asymptotically high frequency initial conditions, with  $\|u_0^\varepsilon\|_{L^2(\mathbb{R}^3)} \leq M$ , then we have*

$$\|\mathcal{P}_t u_0^\varepsilon - P_{t,K}^\varepsilon u_0^\varepsilon\|_{L^2(\mathbb{R}^3)} \lesssim \varepsilon^K M.$$

Please refer to Section 4 and Theorem 4.1 for the formulation of the frozen Gaussian approximation and a precise presentation of the main theorem. The asymptotically high frequency initial condition is defined in Definition 2.2.

**Related works.** The frozen Gaussian approximation is motivated by the Herman-Kluk propagator developed in the chemistry literature [4, 6, 7], which is used in the semiclassical regime of time dependent Schrödinger equation. The convergence of Herman-Kluk propagator was recently proved by Swart and Rouse [20] and Robert [18]. It is proved that the Herman-Kluk propagator converges to the true propagator of the Schrödinger equation. In particular, this means that applied to any initial data in  $L^2$ , the Herman-Kluk propagator provides an accurate result as  $\varepsilon \rightarrow 0$ .

The difference of the Schrödinger equation and the first order hyperbolic system lies in the fact that the hyperbolic system might present singularities at  $p = 0$  on phase plane (see Section 3 for more details). Therefore, one can not hope to obtain similar results for first order hyperbolic system as for Schrödinger equation. Indeed, we construct a counter-example which shows that the method fails to give a good approximation for low frequency initial data in Example 4.2. On the other hand, the results of this work show that frozen Gaussian approximation works for the initial data that are high frequent. This is of course the working assumption for high frequency wave propagation.

The convergence of the Gaussian beam method has been recently investigated in [1, 8–10]. The results in [1, 10] showed that the  $K$ -th order Gaussian beam method converges to the true solution with an accuracy of  $\mathcal{O}(\varepsilon^{K/2})$ . The  $K$ -th order frozen Gaussian approximation, as indicated by Theorem 4.1, has a convergence order  $\mathcal{O}(\varepsilon^K)$ . We refer to [12] for a more detailed numerical comparison between frozen Gaussian approximation and Gaussian beam method.

**Organization of the paper.** In Section 2, we introduce some necessary notations and preliminaries for phase plane analysis. The hyperbolic system we considered is presented in Section 3. Section 4 describes the formulation of frozen Gaussian approximation and states the main convergence theorem. The proof is based on the construction of high order approximate solution given in Section 5 and stability from the well-posedness of hyperbolic system. We conclude the proof in Section 6.

## 2. PRELIMINARIES

**2.1. Notations.** We will in general use  $x, y \in \mathbb{R}^d$  as spatial variables,  $(q, p) \in \mathbb{R}^{2d}$  as the variable for the phase space.  $d$  is the spatial dimensionality. We will use the same notation  $|\cdot|$  for absolute value, Euclidean distance, vector norm, (induced) matrix norm and (induced) tensor norm.

For  $\delta > 0$ , we define the closed set  $K_\delta \subset \mathbb{R}^{2d}$  as

$$(2.1) \quad K_\delta = \left\{ (q, p) \in \mathbb{R}^{2d} \mid |q| \leq 1/\delta, |p| \in [\delta, 1/\delta] \right\}.$$

For  $f : \mathbb{R}^{2d} \rightarrow \mathbb{C}$ , we define for  $k \in \mathbb{N}$  and  $\delta \in \mathbb{R}^+$ ,

$$(2.2) \quad \Lambda_{k,\delta}[f] = \max_{|\alpha| \leq k} \sup_{(q,p) \in K_\delta} \left| \partial^\alpha f(q,p) \right|,$$

where  $\alpha$  is a multi-index. This definition can be extended to vector valued and matrix valued functions straightforwardly.

For  $f : \mathbb{R}^M \rightarrow \mathbb{C}^N$  and  $M, N \in \mathbb{N}$ , the matrix valued function  $\partial_x f : \mathbb{R}^M \rightarrow \mathbb{C}^{M \times N}$  is defined with the convention that  $(\partial_x f(x))_{jk} = \partial_{x_j} f_k(x)$  for  $j = 1, \dots, M$ ,  $k = 1, \dots, N$ .

We use the notations  $\mathcal{S}$ ,  $C^\infty$  and  $C_c^\infty$  for Schwartz function class, smooth functions and compact supported smooth functions respectively.

For convenience, we use the notation  $\mathcal{O}(\varepsilon^\infty)$ :  $A^\varepsilon = \mathcal{O}(\varepsilon^\infty)$  means that for any  $k \in \mathbb{N}$ ,

$$\lim_{\varepsilon \rightarrow 0} \varepsilon^{-k} |A^\varepsilon| = 0.$$

Notations  $c$  and  $C$  will be used for constants, whose values might change from line to line. Sometimes, we will use notations like  $C_{T,K}$  to specify the dependence of the constant on the parameters  $T$  and  $K$ .

**2.2. Wave packet decomposition.** For  $(q, p) \in \mathbb{R}^{2d}$ , define  $\psi_{q,p}^\varepsilon$  as

$$(2.3) \quad \psi_{q,p}^\varepsilon(x) = (2\pi\varepsilon)^{-d/2} \exp\left(ip \cdot (x - q)/\varepsilon - \frac{1}{2}|x - q|^2/\varepsilon\right).$$

Define FBI transform  $\mathcal{F}^\varepsilon$  on  $\mathcal{S}(\mathbb{R}^d)$  as

$$(2.4) \quad \begin{aligned} (\mathcal{F}^\varepsilon f)(q, p) &= (\pi\varepsilon)^{-d/4} \langle \psi_{q,p}^\varepsilon, f \rangle \\ &= 2^{-d/2} (\pi\varepsilon)^{-3d/4} \int_{\mathbb{R}^d} e^{-ip \cdot (x-q)/\varepsilon - \frac{1}{2}|x-q|^2/\varepsilon} f(x) dx. \end{aligned}$$

The inverse FBI transform  $(\mathcal{F}^\varepsilon)^*$  on  $\mathcal{S}(\mathbb{R}^{2d})$  is given by

$$(2.5) \quad ((\mathcal{F}^\varepsilon)^* g)(x) = 2^{-d/2} (\pi\varepsilon)^{-3d/4} \iint_{\mathbb{R}^{2d}} e^{ip \cdot (x-q)/\varepsilon - \frac{1}{2}|x-q|^2/\varepsilon} g(q, p) dq dp.$$

We summarize some elementary properties of the FBI transform, whose proof is standard and can be found, for example, in [13].

**Proposition 2.1.** *For any  $f \in \mathcal{S}(\mathbb{R}^d)$  and  $g \in \mathcal{S}(\mathbb{R}^{2d})$ ,*

$$(2.6) \quad \|\mathcal{F}^\varepsilon f\|_{L^2(\mathbb{R}^{2d})} = \|f\|_{L^2(\mathbb{R}^d)};$$

$$(2.7) \quad \|(\mathcal{F}^\varepsilon)^* g\|_{L^2(\mathbb{R}^d)} = \|g\|_{L^2(\mathbb{R}^{2d})}.$$

Hence, the domain of  $\mathcal{F}^\varepsilon$  and  $(\mathcal{F}^\varepsilon)^*$  can be extended to  $L^2(\mathbb{R}^d)$  and  $L^2(\mathbb{R}^{2d})$  respectively. Moreover, we have

$$(2.8) \quad (\mathcal{F}^\varepsilon)^* \mathcal{F}^\varepsilon = \text{Id}_{L^2(\mathbb{R}^d)}.$$

*Remark.*  $\mathcal{F}^\varepsilon (\mathcal{F}^\varepsilon)^* \neq \text{Id}_{L^2(\mathbb{R}^{2d})}$ .

**Definition 2.2** (Asymptotically high frequency function). Let  $\{u^\varepsilon\} \subset L^2(\mathbb{R}^d)$  be a family of functions such that  $\|u^\varepsilon\|_{L^2}$  is uniformly bounded. Given  $\delta > 0$ , we say that  $\{u^\varepsilon\}$  is *asymptotically high frequency with cutoff  $\delta$* , if

$$\int_{\mathbb{R}^{2d} \setminus K_\delta} |(\mathcal{F}^\varepsilon u^\varepsilon)(q, p)|^2 dq dp = \mathcal{O}(\varepsilon^\infty)$$

as  $\varepsilon \rightarrow 0$ .  $K_\delta$  is the closed set defined in (2.1).

The definition of asymptotically high frequency functions is motivated by WKB function, which is typical in study on high frequency wave propagation.

**Example 2.3.** For  $A(x) \in C_c^\infty(\mathbb{R}^d)$  and  $S(x) \in C^\infty(\mathbb{R}^d)$ ,  $|\nabla S(x)| \geq \delta > 0$ , the family of WKB functions  $u^\varepsilon = A(x) \exp(iS(x)/\varepsilon)$  is asymptotically high frequency with cutoff  $\delta$ .

The Definition 2.2 is also related with the notion of frequency set, microlocal support in microlocal analysis. Please refer to [13] for more details.

## 3. HYPERBOLIC SYSTEM AND HAMILTONIAN FLOW

We consider an  $N \times N$  linear hyperbolic system in  $d$  dimensional space,

$$(3.1) \quad \partial_t u + \sum_{l=1}^d A_l(x) \partial_{x_l} u = 0,$$

where  $u = (u_1, \dots, u_N)^T : \mathbb{R}^d \rightarrow \mathbb{R}^N$  and  $A_l : \mathbb{R}^d \rightarrow \mathbb{R}^{N \times N}$ ,  $1 \leq l \leq d$  are smooth matrix valued functions.

We assume that the system (3.1) is *strictly hyperbolic*, i.e., for any  $(q, p) \in \mathbb{R}^{2d}$ ,  $|p| > 0$ , the matrix  $\sum_{l=1}^d p_l A_l(q)$  has  $N$  *distinguished* real eigenvalues, denoted as  $\{H_n(q, p)\}_{n=1}^N$ . We denote by  $L_n(q, p)$  and  $R_n(q, p)$  the corresponding left and right eigenvectors, i.e.,

$$(3.2) \quad \sum_{l=1}^d p_l L_n^T(q, p) A_l(q) = H_n(q, p) L_n^T(q, p),$$

$$(3.3) \quad \sum_{l=1}^d p_l A_l(q) R_n(q, p) = H_n(q, p) R_n(q, p),$$

with the normalization

$$L_m^T(q, p) R_n(q, p) = \delta_{mn},$$

where  $\delta_{mn}$  is the Kronecker symbol. Note that as  $A_l(q)$  is smooth,  $H_n(q, p)$ ,  $R_n(q, p)$  and  $L_n(q, p)$  are smooth functions of  $(q, p)$  for  $|p| > 0$ . Singularities may occur at  $p = 0$ .

The Hamiltonian flow associated with  $H_n(q, p)$  is given for  $|p| > 0$  as

$$(3.4) \quad \begin{cases} \frac{dQ_n(t, q, p)}{dt} = \partial_{P_n} H_n(Q_n(t, q, p), P_n(t, q, p)), \\ \frac{dP_n(t, q, p)}{dt} = -\partial_{Q_n} H_n(Q_n(t, q, p), P_n(t, q, p)), \end{cases}$$

with initial conditions

$$(3.5) \quad Q_n(0, q, p) = q \quad \text{and} \quad P_n(0, q, p) = p.$$

This gives the map  $(q, p) \mapsto (Q_n(t, q, p), P_n(t, q, p))$  for both  $t > 0$  and  $t < 0$  (forward and backward flows). For  $p = 0$  and  $q \in \mathbb{R}^d$ , we define  $Q_n(t, q, p) = q$  and  $P_n(t, q, p) = p$ .

We make the following assumption for the system (3.1) we consider, which will be assumed for the rest of the paper without further indication.

**Assumption A.** For each  $n = 1, \dots, N$ , there exists constant  $C > 0$ , so that the Hamiltonian  $H_n$  satisfies for any  $(q, p) \in \mathbb{R}^{2d}$  with  $|p| > 0$

$$|p \cdot \partial_q H_n(q, p)| \leq C |p|^2, \quad \text{and} \quad |q \cdot \partial_p H_n(q, p)| \leq C |q|^2.$$

Assumption A is understood as a global Lipschitz condition for the ODEs (3.4), as we can see from the next Proposition.

**Proposition 3.1.** *For each  $n = 1, \dots, N$ ,  $T > 0$  and  $\delta > 0$ , there exists a constant  $\delta_T > 0$  such that  $(Q_n(t, q, p), P_n(t, q, p)) \in K_{\delta_T}$ , i.e., it satisfies*

$$(3.6) \quad \delta_T \leq |P_n(t, q, p)| \leq 1/\delta_T,$$

and

$$(3.7) \quad |Q_n(t, q, p)| \leq 1/\delta_T,$$

for any  $(q, p) \in K_\delta$  and  $t \in [0, T]$ .

*Proof.* We suppress the subscript  $n$  in the proof, since the argument is the same for each branch.

Differentiating  $|P|$  with respect to time and using (3.4) produce

$$\frac{d}{dt} |P| = \frac{1}{|P|} P \cdot \frac{d}{dt} P = -\frac{1}{|P|} P \cdot \partial_Q H.$$

Hence, by Assumption A,

$$\frac{d}{dt} |P| \leq \frac{1}{|P|} |P \cdot \partial_Q H| \leq C |P|.$$

Gronwall's inequality implies

$$\max_{0 \leq t \leq T} |P(t, q, p)| \leq C_T |p|.$$

On the other hand, differentiating  $|P|^{-1}$  gives

$$\frac{d}{dt} \left( \frac{1}{|P|} \right) = \frac{1}{|P|^3} P \cdot \partial_Q H.$$

This yields

$$\frac{d}{dt} \left( \frac{1}{|P|} \right) \leq \frac{1}{|P|^3} |P \cdot \partial_Q H| \leq C \frac{1}{|P|},$$

and hence

$$\max_{0 \leq t \leq T} |P(t, q, p)|^{-1} \leq C_T |p|^{-1}.$$

Therefore, there exist  $c_T, C_T > 0$  such that for  $t \in [0, T]$  and any  $q \in \mathbb{R}^d$ ,

$$c_T |p| \leq |P(t, q, p)| \leq C_T |p|,$$

which implies (3.6).

The time derivative of  $|Q|$  can be bounded by

$$\frac{d}{dt} |Q| = \frac{1}{|Q|} Q \cdot \partial_P H \leq C |Q|$$

by Assumption A. Equation (3.7) then follows from Gronwall's inequality.  $\square$

**Proposition 3.2.** *For  $l = 1, \dots, d$ ,  $k \in \mathbb{N}$  and  $\delta > 0$ , there exists constant  $C_{k,\delta}$  such that*

$$\Lambda_{k,\delta}[A_l] \leq C_{k,\delta}.$$

Moreover, for each  $n = 1, \dots, N$ , there exists constant  $C_{k,\delta}$  such that

$$\Lambda_{k,\delta}[H_n] \leq C_{k,\delta}, \quad \Lambda_{k,\delta}[R_n] \leq C_{k,\delta}, \quad \Lambda_{k,\delta}[L_n] \leq C_{k,\delta}.$$

*Proof.* The conclusion follows immediately from the smoothness of  $A_l, H_n, R_n, L_n$  for  $|p| > 0$  and the compactness of the set  $K_\delta$ .  $\square$

We define canonical transformation and action associated with Hamiltonian flow.

**Definition 3.3** (Canonical transformation). Let

$$(3.8) \quad \begin{aligned} & \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d} \\ \kappa : & (q, p) \mapsto (Q^\kappa(q, p), P^\kappa(q, p)) \end{aligned}$$

be differentiable for  $|p| > 0$ . We denote the Jacobian matrix as

$$(3.9) \quad F^\kappa(q, p) = \begin{pmatrix} (\partial_q Q^\kappa)^\top(q, p) & (\partial_p Q^\kappa)^\top(q, p) \\ (\partial_q P^\kappa)^\top(q, p) & (\partial_p P^\kappa)^\top(q, p) \end{pmatrix}.$$

We say  $\kappa$  is a *canonical transformation* if  $F^\kappa$  is symplectic for any  $(q, p) \in \mathbb{R}^{2d}$  with  $|p| > 0$ ,

$$(3.10) \quad (F^\kappa)^\top \begin{pmatrix} 0 & \text{Id}_d \\ -\text{Id}_d & 0 \end{pmatrix} F^\kappa = \begin{pmatrix} 0 & \text{Id}_d \\ -\text{Id}_d & 0 \end{pmatrix}.$$

As a corollary to Proposition 3.2, the map  $\kappa_{n,t} : (q, p) \mapsto (Q_n(t, q, p), P_n(t, q, p))$  is a canonical transformation. We formulate this as the next proposition, which also gives additional smoothness properties for the Jacobian.

**Proposition 3.4.** *For each  $n = 1, \dots, N$ , the map  $\kappa_{n,t}$  is a canonical transformation, and for any  $k \geq 0$ ,  $\delta > 0$  and  $T > 0$ , there exists constant  $C_{k,\delta,T}$  such that*

$$(3.11) \quad \sup_{t \in [0, T]} \Lambda_{k,\delta}[F^{\kappa_{n,t}}] \leq C_{k,\delta,T}.$$

*Proof.* The argument is the same for different branches, hence we will suppress the subscript  $n$  for simplicity.

Proposition 3.1 shows that there exists  $\delta_T$  such that  $(Q(t, q, p), P(t, q, p)) \in K_{\delta_T}$  for  $(q, p) \in K_\delta$  and  $t \in [0, T]$ .

Differentiating  $F^{\kappa_t}(q, p)$  with respect to time gives

$$(3.12) \quad \frac{d}{dt} F^{\kappa_t}(q, p) = \begin{pmatrix} \partial_P \partial_Q H & \partial_P \partial_P H \\ -\partial_Q \partial_Q H & -\partial_Q \partial_P H \end{pmatrix} F^{\kappa_t}(q, p).$$

Proposition 3.1 and 3.2 imply

$$\frac{d}{dt} |F^{\kappa_t}(q, p)| = \left| \begin{pmatrix} \partial_P \partial_Q H & \partial_P \partial_P H \\ -\partial_Q \partial_Q H & -\partial_Q \partial_P H \end{pmatrix} \right| |F^{\kappa_t}(q, p)| \leq C |F^{\kappa_t}(q, p)|,$$

where  $C$  is independent of  $(q, p)$ . Hence, by Gronwall's inequality and  $F^{\kappa_0}(q, p) = \text{Id}_{2d}$ , one has

$$|F^{\kappa_t}(q, p)| \leq \exp(C|t|).$$

Differentiating (3.12) with  $(q, p)$  yields

$$\frac{d}{dt} \partial_{(q,p)}^\alpha F^{\kappa_t}(q, p) = \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} \partial_{(q,p)}^\beta \begin{pmatrix} \partial_P \partial_Q H & \partial_P \partial_P H \\ -\partial_Q \partial_Q H & -\partial_Q \partial_P H \end{pmatrix} \partial_{(q,p)}^{\alpha-\beta} F^{\kappa_t}(q, p).$$

The estimate (3.11) follows by an induction argument.  $\square$

**Definition 3.5** (Action). Let  $\kappa$  be a canonical transformation defined in (3.8). A function  $S^\kappa : \mathbb{R}^{2d} \rightarrow \mathbb{R}$  is called an *action associated to  $\kappa$*  if it satisfies

$$(3.13) \quad \partial_p S^\kappa(q, p) = (\partial_p Q^\kappa(q, p)) P^\kappa(q, p),$$

$$(3.14) \quad \partial_q S^\kappa(q, p) = -p + (\partial_q Q^\kappa(q, p)) P^\kappa(q, p),$$

for any  $|p| > 0$ .

The action  $S_n(t, q, p) = S^{\kappa_{n,t}}(q, p)$  corresponding to  $H_n(q, p)$  solves the following equation

$$(3.15) \quad \frac{dS_n}{dt} = P_n \cdot \partial_P H_n(P_n, Q_n) - H_n(P_n, Q_n),$$

with initial condition  $S_n(t, q, p) = 0$ . It is easy to check that  $S_n$  is indeed the action associated with  $\kappa_{n,t}$ , which is given by

$$(3.16) \quad S_n(t, q, p) = \int_0^t P_n(\tau, q, p) \cdot \partial_\tau Q_n(\tau, q, p) - H_n(Q_n(\tau, q, p), P_n(\tau, q, p)) d\tau.$$

Now we are ready to construct the Fourier integral operator which will be used in the definition of frozen Gaussian approximation in the next section.

**Definition 3.6** (Fourier Integral Operator). For  $M \in L^\infty(\mathbb{R}^{2d}; \mathbb{C}^{N \times N})$ , a Schwartz-class function  $u \in \mathcal{S}(\mathbb{R}^d; \mathbb{C}^N)$  and  $n = 1, \dots, N$ , we define

$$(3.17) \quad (\mathcal{I}_n^\varepsilon(t, M)u)(x) = (2\pi\varepsilon)^{-3d/2} \int_{\mathbb{R}^{3d}} e^{i\Phi_n(t,x,y,q,p)/\varepsilon} M(q, p) u(y) dq dp dy.$$

where the phase function  $\Phi_n$  is given by

$$(3.18) \quad \begin{aligned} \Phi_n(t, x, y, q, p) = S_n(t, q, p) + \frac{i}{2} |x - Q_n(t, q, p)|^2 + P_n \cdot (x - Q_n(t, q, p)) \\ + \frac{i}{2} |y - q|^2 - p \cdot (y - q). \end{aligned}$$



**Proposition 3.7.** *If  $M \in L^\infty(\mathbb{R}^{2d}; \mathbb{C}^{N \times N})$ , for each  $n = 1, \dots, N$  and any  $t$ ,  $\mathcal{I}_n^\varepsilon(t, M)$  can be extended to a linear bounded operator on  $L^2(\mathbb{R}^d; \mathbb{C}^N)$ , and we have*

$$(3.19) \quad \|\mathcal{I}_n^\varepsilon(t, M)\|_{\mathcal{L}(L^2(\mathbb{R}^d; \mathbb{C}^N))} \leq 2^{-d/2} \|M\|_{L^\infty(\mathbb{R}^{2d}; \mathbb{C}^{N \times N})}.$$

*Proof.* For  $u, v \in L^2(\mathbb{R}^d)$ , taking the inner product of  $v$  and (3.17) gives

$$\begin{aligned} \langle v, \mathcal{I}_n^\varepsilon(t, M)u \rangle &= (2\pi\varepsilon)^{-3d/2} \int_{\mathbb{R}^{4d}} v(x)^* e^{i\Phi_n(t, x, y, q, p)/\varepsilon} M(q, p) u(y) \, dq \, dp \, dy \, dx \\ &= (2\pi\varepsilon)^{-3d/2} \int_{\mathbb{R}^{2d}} dq \, dp \, e^{iS_n(t, q, p)/\varepsilon} \\ &\quad \times \overline{\left( \int_{\mathbb{R}^d} e^{-\frac{i}{\varepsilon} P_n \cdot (x - Q_n) - \frac{1}{2\varepsilon} |x - Q_n|^2} v(x) \, dx \right)} \\ &\quad \times M(q, p) \int_{\mathbb{R}^d} e^{-\frac{i}{\varepsilon} p \cdot (y - q) - \frac{1}{2\varepsilon} |y - q|^2} u(y) \, dy \\ &= 2^{-d/2} \int_{\mathbb{R}^{2d}} e^{iS_n(t, q, p)/\varepsilon} \overline{(\mathcal{F}^\varepsilon v)}(Q_n, P_n) M(q, p) (\mathcal{F}^\varepsilon u)(q, p) \, dq \, dp. \end{aligned}$$

Therefore,

$$\begin{aligned} |\langle v, \mathcal{I}_n^\varepsilon(t, M)u \rangle| &\leq 2^{-d/2} \|(\mathcal{F}^\varepsilon v) \circ \kappa_{n,t}\|_{L^2(\mathbb{R}^{2d}; \mathbb{C}^N)} \left\| e^{iS_n/\varepsilon} M(\mathcal{F}^\varepsilon u) \right\|_{L^2(\mathbb{R}^{2d}; \mathbb{C}^N)} \\ &\leq 2^{-d/2} \|v\|_{L^2(\mathbb{R}^d; \mathbb{C}^N)} \|M\|_{L^\infty(\mathbb{R}^{2d}; \mathbb{C}^{N \times N})} \|u\|_{L^2(\mathbb{R}^d; \mathbb{C}^N)}, \end{aligned}$$

where we have used Proposition 2.1 and the symplecticity of the canonical transform  $\kappa_{n,t}$ . This implies

$$\|\mathcal{I}_n^\varepsilon(t, M)u\|_{L^2(\mathbb{R}^d; \mathbb{C}^N)} \leq 2^{-d/2} \|M\|_{L^\infty(\mathbb{R}^{2d}; \mathbb{C}^{N \times N})} \|u\|_{L^2(\mathbb{R}^d; \mathbb{C}^N)},$$

which proves the Proposition.  $\square$

#### 4. FORMULATION AND MAIN RESULT

Let  $\chi_\delta : \mathbb{R}^{2d} \rightarrow [0, 1]$  be a smooth cutoff function for  $\delta > 0$  so that

$$\chi_\delta(q, p) = \begin{cases} 1, & (q, p) \in K_\delta; \\ 0, & (q, p) \in \mathbb{R}^{2d} \setminus K_{\delta/2}, \end{cases}$$

and for any  $k \in N$ , there exists constant  $C_{k,\delta}$  such that

$$\sup_{(q,p) \in \mathbb{R}^{2d}} \sup_{|\alpha|=k} \left| \partial_{(q,p)}^\alpha \chi_\delta(q, p) \right| \leq C_{k,\delta}.$$

The construction of the cutoff function is standard.

Construct the  $K$ -th order frozen Gaussian approximation with the cutoff  $\delta$  as

$$\begin{aligned} (\mathcal{P}_{t,K,\delta}^\varepsilon u_0)(x) &= \sum_{n=1}^N (\mathcal{I}_n^\varepsilon(t, \mathcal{M}_{n,K,t}^\varepsilon \chi_\delta) u_0)(x) \\ &= \frac{1}{(2\pi\varepsilon)^{3d/2}} \sum_{n=1}^N \int_{\mathbb{R}^{3d}} e^{i\Phi_n/\varepsilon} \mathcal{M}_{n,K,t}^\varepsilon(q, p) \chi_\delta(q, p) u_0(y) \, dq \, dp \, dy. \end{aligned}$$

Here, the matrix symbol  $\mathcal{M}_{n,K,t}^\varepsilon$  is given by

$$(4.2) \quad \mathcal{M}_{n,K,t}^\varepsilon(q,p) = \mathcal{M}_{n,K}^\varepsilon(t,q,p) = \sum_{k=0}^{K-1} \varepsilon^k M_{n,k}(t,q,p).$$

Before we introduce the  $N \times N$  matrix valued function  $M_{n,k}(t,q,p)$ , we need to define some operators first. We denote

$$(4.3) \quad \partial_z = \partial_q - \iota \partial_p, \quad Z_n(t,q,p) = \partial_z (Q_n(t,q,p) + \iota P_n(t,q,p)).$$

Note that  $Z_n(t,q,p)$  is invertible for  $|p| > 0$ , which will be proved in Lemma 5.1. Without further indication, we are going to use the Einstein summation convention, except for the branch index  $n$ .

We denote  $b : \mathbb{R}^{2d} \rightarrow \mathbb{C}$  as a generic function defined on  $\mathbb{R}^{2d}$ . For indices  $j_1, j_2 \in \{1, \dots, d\}$ , define operators  $\mathcal{D}$  and  $\mathcal{G}$  as

$$(4.4) \quad (\mathcal{D}_{n,j_1} b)(q,p) = -\partial_{z_i} (b(q,p) Z_{n,j_1 i}^{-1}(t,q,p)),$$

$$(4.5) \quad (\mathcal{G}_{n,j_1 j_2} b)(q,p) = \partial_{z_i} Q_{n,j_1}(t,q,p) b(q,p) Z_{n,j_2 i}^{-1}(t,q,p),$$

provided the right hand sides are well defined (in particular,  $b$  is differentiable at  $(q,p)$ ).

For  $\nu \in \mathbb{N}$ ,  $j_\alpha \in \{1, \dots, d\}$  for  $\alpha = 1, \dots, \nu$ , and  $\varepsilon > 0$ , define operators  $\mathcal{T}_{n,j_1 \dots j_\nu}^{\nu, \varepsilon}$  as

$$(4.6) \quad \mathcal{T}_{n,j_1}^{1, \varepsilon} b = \varepsilon \mathcal{D}_{n,j_1} b,$$

$$(4.7) \quad \mathcal{T}_{n,j_1 j_2}^{2, \varepsilon} b = \varepsilon \mathcal{G}_{n,j_1 j_2} b + \varepsilon^2 \mathcal{D}_{n,j_1} \mathcal{D}_{n,j_2} b,$$

and for  $\nu \geq 3$ ,

$$(4.8) \quad \mathcal{T}_{n,j_1 \dots j_\nu}^{\nu, \varepsilon} b = \varepsilon \mathcal{T}_{n,j_1 \dots j_{\nu-1}}^{\nu-1, \varepsilon} \mathcal{D}_{n,j_\nu} b + \varepsilon \sum_{\alpha=1}^{\nu-1} \mathcal{T}_{n,j_1 \dots j_{\alpha-1} j_{\alpha+1} \dots j_{\nu-1}}^{\nu-2, \varepsilon} \mathcal{G}_{n,j_\alpha j_\nu} b,$$

provided the right hand sides are well defined at  $(q,p) \in \mathbb{R}^{2d}$ . Notice that  $\mathcal{D}$ ,  $\mathcal{G}$  and  $\mathcal{T}$  depend on  $t$  as well, which we choose not to make explicit in notation for simplicity, with the hope that no confusion will occur.

It is easy to see that we can rewrite  $\mathcal{T}_{n,j_1 \dots j_\nu}^{\nu, \varepsilon}$  in orders of  $\varepsilon$  as

$$(4.9) \quad \mathcal{T}_{n,j_1 \dots j_\nu}^{\nu, \varepsilon} b = \sum_{k=\lceil \nu/2 \rceil}^{\nu} \varepsilon^k \mathcal{T}_{n,j_1 \dots j_\nu}^{\nu, k} b,$$

where  $\lceil \cdot \rceil$  is the ceiling function. The last equality defines  $\mathcal{T}_{n,j_1 \dots j_\nu}^{\nu, k}$ . The definition of these operators  $\mathcal{D}$ ,  $\mathcal{G}$  and  $\mathcal{T}$  can be extended to vector-valued and matrix-valued functions so that the operators act on the function elementwisely. For example, for the matrix-valued function  $M : \mathbb{R}^{2d} \rightarrow \mathbb{C}^{N \times N}$ , we have

$$(\mathcal{D}_{n,j_1} M)_{kl} = \mathcal{D}_{n,j_1} M_{kl},$$

for  $k, l = 1, \dots, N$ .

We define the operator  $\mathcal{L}_{n,k}$  as follows. For  $M : \mathbb{R} \times \mathbb{R}^{2d} \rightarrow \mathbb{C}^{N \times N}$  and  $(t, q, p) \in \mathbb{R} \times \mathbb{R}^{2d}$  with  $|p| > 0$ ,  $\mathcal{L}_{n,k}(M)$  is given by

$$(4.10) \quad \begin{aligned} (\mathcal{L}_{n,0}M)(t, q, p) &= \imath \left( \partial_t S_n - P_{n,j} \partial_t Q_{n,j} + P_{n,j} A_j(Q_n) \right) M(t, q, p) \\ &= \imath \left( P_{n,j} A_j(Q_n) - H_n(Q_n, P_n) \text{Id}_N \right) M(t, q, p), \end{aligned}$$

$$(4.11) \quad \begin{aligned} (\mathcal{L}_{n,1}M)(t, q, p) &= \partial_t M(t, q, p) \\ &\quad + \imath \mathcal{D}_{n,j} \left( \left( (\partial_t P_{n,j} - \imath \partial_t Q_{n,j}) \text{Id}_N \right. \right. \\ &\quad \left. \left. + \imath A_j(Q_n) + P_{n,l} \partial_j A_l(Q_n) \right) M(t, q, p) \right) \\ &\quad + \imath \mathcal{G}_{n,j_1 j_2} \left( \left( \imath \partial_{Q_{n,j_1}} A_{j_2}(Q_n) \right. \right. \\ &\quad \left. \left. + \frac{1}{2} P_{n,l} \partial_{j_1 j_2}^2 A_l(Q_n) \right) M(t, q, p) \right), \end{aligned}$$

where  $S_n, Q_n$  and  $P_n$  on the right hand sides are evaluated at  $(t, q, p)$  and we have introduced the short-hand,

$$\partial_{j_1 \dots j_\nu}^\nu A_l(Q_n) = \partial_{Q_{n,j_1} \dots Q_{n,j_\nu}}^\nu A_l(Q_n), \quad \text{for any } \nu \geq 1.$$

Moreover, for  $k \geq 2$ , we define

$$(4.12) \quad \begin{aligned} (\mathcal{L}_{n,k}M)(t, q, p) &= \sum_{\nu=k}^{2k} \mathcal{T}_{n,j_1 \dots j_\nu}^{\nu,k} \left( \left( -\frac{1}{(\nu-1)!} \partial_{j_1 \dots j_{\nu-1}}^{\nu-1} A_{j_\nu}(Q_n) \right. \right. \\ &\quad \left. \left. + \frac{\imath}{\nu!} P_{n,l} \partial_{j_1 \dots j_\nu}^\nu A_l(Q_n) \right) M(t, q, p) \right). \end{aligned}$$

We remind the readers that  $\mathcal{D}$ ,  $\mathcal{G}$  and  $\mathcal{T}$  depend on  $t$  implicitly.

We are ready to give the matrix-valued function  $M_{n,k}$  now.  $M_{n,k}$  is defined for  $t \in [0, T]$  and  $(q, p) \in \mathbb{R}^{2d}$  with  $|p| > 0$ . First,  $M_{n,0}$  is given by

$$(4.13) \quad M_{n,0}(t, q, p) = \sigma_{n,0}(t, q, p) R_n(Q_n(t, q, p), P_n(t, q, p)) L_n(q, p)^\text{T},$$

where  $\sigma_{n,0}$  is determined by the evolution equation,

$$(4.14) \quad \frac{d}{dt} \sigma_{n,0}(t, q, p) + \sigma_{n,0}(t, q, p) \lambda_n(t, q, p) = 0,$$

with the initial condition

$$(4.15) \quad \sigma_{n,0}(0, q, p) = 2^{d/2}.$$

In (4.14), we have used the short-hand

$$(4.16) \quad \begin{aligned} \lambda_n(t, q, p) &= L_n^\text{T} (\partial_{P_n} H_n \cdot \partial_{Q_n} R_n - \partial_{Q_n} H_n \cdot \partial_{P_n} R_n) \\ &\quad - (\partial_{z_k} L_n)^\text{T} \left( (A_j - \partial_{P_{n,j}} H_n) + \imath (\partial_{Q_{n,j}} H_n - P_{n,l} \partial_j A_l) \right) R_n Z_{n,jk}^{-1} \\ &\quad + \partial_{z_s} Q_{n,j} Z_{n,ks}^{-1} L_n^\text{T} (-\partial_j A_k + \frac{\imath}{2} P_{n,l} \partial_{jk}^2 A_l) R_n, \end{aligned}$$

where  $Q_n, P_n$  are evaluated at  $(t, q, p)$ ,  $A_j$ 's are evaluated at  $Q_n$ , and  $H_n, L_n, R_n$  are evaluated at  $(Q_n, P_n)$ .

Notice that the action  $\mathcal{L}_{n,0}$  is just multiplication with the matrix  $\iota(P_{n,j}A_j(Q_n) - H_n(Q_n, P_n)\text{Id}_N)$  on the left. We define the matrix,

$$(4.17) \quad \mathcal{L}_{n,0}^\dagger(q, p) = \iota \sum_{m \neq n} (H_n(q, p) - H_m(q, p))^{-1} R_m(q, p) L_m^\top(q, p).$$

For  $k \geq 1$ ,  $M_{n,k}$  is given by

$$(4.18) \quad M_{n,k}(t, q, p) = \sigma_{n,k}(t, q, p) R_n(Q_n(t, q, p), P_n(t, q, p)) L_n(q, p)^\top + M_{n,k}^\perp(t, q, p),$$

where  $M_{n,k}^\perp(t, q, p)$  is given by

$$(4.19) \quad M_{n,k}^\perp(t, q, p) = \mathcal{L}_{n,0}^\dagger(Q_n(t, q, p), P_n(t, q, p)) \sum_{s=1}^k (\mathcal{L}_{n,s} M_{n,k-s})(t, q, p),$$

and  $\sigma_{n,k}(t, q, p)$  solves

$$(4.20) \quad \frac{d\sigma_{n,k}}{dt} + \sigma_{n,k} \lambda_n + L_n(Q_n(t, q, p), P_n(t, q, p))^\top \left( (\mathcal{L}_{n,1} M_{n,k}^\perp)(t, q, p) + \sum_{s=2}^{k+1} (\mathcal{L}_{n,s} M_{n,k+1-s})(t, q, p) \right) R_n(q, p) = 0,$$

with the initial condition  $\sigma_{n,k}(0, q, p) = 0$ .

We now state the main result. The following theorem indicates that the  $K$ -th order frozen Gaussian approximation (FGA) gives an order  $\mathcal{O}(\varepsilon^K)$  approximate solution to strictly linear hyperbolic system.

**Theorem 4.1.** *Consider a strictly linear hyperbolic system (3.1) under Assumption A. For a family of initial conditions  $\{u_0^\varepsilon\}$  that is asymptotically high frequency with cutoff  $\delta$ , and  $\|u_0^\varepsilon\|_{L^2(\mathbb{R}^d)} \leq M$ , then for any  $T > 0$  and  $K \in \mathbb{N}$ , there exist constants  $C_{T,K}$  and  $\varepsilon_0 > 0$ , such that for  $\varepsilon \in (0, \varepsilon_0]$ ,*

$$\max_{0 \leq t \leq T} \|\mathcal{P}_t u_0^\varepsilon - \mathcal{P}_{t,K,\delta}^\varepsilon u_0^\varepsilon\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \leq C_{T,K} M \varepsilon^K.$$

*Remark.* The cutoff  $\delta$  is used in the formulation to avoid singularities presented at  $|p| = 0$ . From an numerical point of view, the cutoff is quite natural. Indeed, in the numerical implementation of frozen Gaussian approximation [11, 12], a cutoff on phase plane is always used for efficiency.

*Remark.* The necessity of assumption that the initial value is asymptotically high frequency is presented in the following example. It shows that the FGA does not work if the FBI transform of the initial condition concentrates around  $|p| = 0$  as  $\varepsilon \rightarrow 0$ .

**Example 4.2.** Consider the acoustic wave equation in two dimension with constant coefficients,

$$\partial_t u + A_1 \partial_{x_1} u + A_2 \partial_{x_2} u = 0,$$

where

$$A_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

Then the eigenfunctions in (3.2)-(3.3) are given by

$$H_1(q, p) = 0, \quad H_{\pm}(q, p) = \pm |p|,$$

where we have used the subscripts  $\pm$  instead of number subscripts. This implies the system is strictly hyperbolic, and the corresponding eigenvectors are

$$R_1(q, p) = \begin{pmatrix} p_2 \\ -p_1 \\ 0 \end{pmatrix}, \quad R_{\pm}(q, p) = \begin{pmatrix} \pm p_1 \\ \pm p_2 \\ |p| \end{pmatrix},$$

$$L_1(q, p) = \frac{1}{|p|^2} \begin{pmatrix} p_2 \\ -p_1 \\ 0 \end{pmatrix}, \quad L_{\pm}(q, p) = \frac{1}{2} \begin{pmatrix} \pm p_1 / |p|^2 \\ \pm p_2 / |p|^2 \\ 1 / |p| \end{pmatrix}.$$

It is easy to see that the system satisfies Assumption A.

We focus on the “+” branch and omit the subscript “+” for convenience, then the Hamiltonian flow is given by

$$(4.21) \quad \begin{cases} \frac{dQ}{dt} = \frac{P}{|P|}, \\ \frac{dP}{dt} = 0, \end{cases}$$

with the initial conditions  $Q(0, q, p) = q$  and  $P(0, q, p) = p$ , which implies the following solution,

$$(4.22) \quad Q = q + \frac{p}{|p|} t, \quad P = p.$$

Therefore

$$(4.23) \quad Z = 2\text{Id}_2 - \frac{it}{|p|} \left( \text{Id}_2 - \frac{p \otimes p}{|p|^2} \right), \quad \det Z = 4 - \frac{2it}{|p|}.$$

According to the equation (2.7) in [12], the solution of amplitude  $\sigma(t, q, p)$  is

$$(4.24) \quad \sigma = \left( 4 - \frac{2it}{|p|} \right)^{1/2},$$

with the branch of square root determined continuously in time by initial condition.

If we take the initial condition of  $u$  as

$$(4.25) \quad u_0(x) = (u_{0,1}, u_{0,2}, u_{0,3})^T = (\exp(-|x|^2/2), 0, 0)^T,$$

then the FBI transform gives

$$(4.26) \quad \begin{aligned} \mathcal{F}^\varepsilon(u_{0,1}) &= \frac{1}{(\pi\varepsilon)^{1/2}(1+\varepsilon)} \exp\left(\frac{ip \cdot q}{1+\varepsilon} - \frac{|q|^2}{2(1+\varepsilon)} - \frac{|p|^2}{2\varepsilon(1+\varepsilon)}\right), \\ \mathcal{F}^\varepsilon(u_{0,2}) &= 0, \\ \mathcal{F}^\varepsilon(u_{0,3}) &= 0. \end{aligned}$$

The leading order frozen Gaussian approximation of  $u$  is given by

$$(4.27) \quad u^\varepsilon(t, x) = \frac{1}{2}(\mathcal{F})^*(\sigma(t, q, p)R(Q, P)L^T(q, p)\mathcal{F}^\varepsilon(u_0)),$$

By Proposition 2.1,

$$(4.28) \quad \begin{aligned} \|u^\varepsilon\|_{L^2}^2 &= \left\| \frac{1}{2}\sigma(t, q, p)R(Q, P)L^T(q, p)\mathcal{F}^\varepsilon(u_0) \right\|_{L^2}^2 \\ &= \frac{1}{(\pi\varepsilon)(1+\varepsilon)^2} \int_{\mathbb{R}^4} \left| 1 - \frac{it}{2|p|} \right| \frac{p_1^4}{4|p|^4} \exp\left(-\frac{|q|^2}{1+\varepsilon} - \frac{|p|^2}{\varepsilon(1+\varepsilon)}\right) dq dp. \end{aligned}$$

Notice that, as  $\varepsilon \rightarrow 0$ ,

$$\int_{\mathbb{R}^2} e^{-\frac{|q|^2}{1+\varepsilon}} dq = \mathcal{O}(1),$$

and

$$\begin{aligned} \frac{1}{\varepsilon} \int_{\mathbb{R}^2} \left| 1 - \frac{it}{2|p|} \right| \frac{p_1^4}{4|p|^4} e^{-\frac{|p|^2}{\varepsilon(1+\varepsilon)}} dp &= \frac{1}{\varepsilon} \int_0^\infty \int_0^{2\pi} \left| 1 - \frac{it}{2r} \right| \frac{\cos^4 \theta}{4} e^{-\frac{r^2}{\varepsilon(1+\varepsilon)}} r dr d\theta, \\ &= \frac{1}{\sqrt{\varepsilon}} \int_0^\infty \int_0^{2\pi} \left| \sqrt{\varepsilon}r - \frac{it}{2} \right| \frac{\cos^4 \theta}{4} e^{-\frac{r^2}{(1+\varepsilon)}} dr d\theta \\ &= \mathcal{O}(\varepsilon^{-1/2}), \end{aligned}$$

where the second equality is obtained by change of variable.

Hence one has  $\|u^\varepsilon\|_{L^2}$  is of the order  $\mathcal{O}(\varepsilon^{-1/4})$ , while  $\|u\|_{L^2}$  under the initial condition (4.25) is of the order  $\mathcal{O}(1)$ , which implies FGA can not be a good approximation to the acoustic wave equation under this choice of initial condition.

## 5. HIGH ORDER APPROXIMATION

In this section we introduce a high order approximation to the solution of (3.1) based on frozen Gaussian approximation. This is a key step in the proof of Theorem 4.1. We state and prove some preliminary lemmas first.

For a canonical transformation  $\kappa_{n,t}$ , define  $Z^{\kappa_{n,t}}(q, p)$  for  $|p| > 0$  as

$$Z^{\kappa_{n,t}}(q, p) = \partial_z(Q^{\kappa_{n,t}}(q, p) + \iota P^{\kappa_{n,t}}(q, p)),$$

which is related to  $Z_n(t, q, p)$  defined in (4.3) by

$$Z_n(t, q, p) = Z^{\kappa_{n,t}}(q, p).$$

**Lemma 5.1.**  $Z^{\kappa_{n,t}}(q, p)$  is invertible for each  $n = 1, \dots, N$  and  $(q, p) \in \mathbb{R}^{2d}$  with  $|p| > 0$ . Moreover, for any  $k \geq 0$  and  $\delta > 0$ , there exists constant  $C_{k,\delta}$  such that

$$(5.1) \quad \Lambda_{k,\delta}[(Z^{\kappa_{n,t}})^{-1}(q, p)] \leq C_{k,\delta}.$$

*Proof.* Since the proof is the same for each branch, we omit the subscript  $n$  in notation for convenience.

Observe that  $Z^{\kappa_t}(q, p)$  can be rewritten as

$$Z^{\kappa_t}(q, p) = \partial_z(Q^{\kappa_t}(q, p) + \iota P^{\kappa_t}(q, p)) = \begin{pmatrix} \iota \text{Id}_d & \text{Id}_d \end{pmatrix} (F^{\kappa_t})^\top(q, p) \begin{pmatrix} -\iota \text{Id}_d \\ \text{Id}_d \end{pmatrix}.$$

Therefore,

$$\begin{aligned} (Z^{\kappa_t}(Z^{\kappa_t})^*)(q, p) &= \begin{pmatrix} \iota \text{Id}_d & \text{Id}_d \end{pmatrix} (F^{\kappa_t})^\top(q, p) \begin{pmatrix} \text{Id}_d & -\iota \text{Id}_d \\ \iota \text{Id}_d & \text{Id}_d \end{pmatrix} F^{\kappa_t}(q, p) \begin{pmatrix} -\iota \text{Id}_d \\ \text{Id}_d \end{pmatrix} \\ &= \begin{pmatrix} \iota \text{Id}_d & \text{Id}_d \end{pmatrix} ((F^{\kappa_t})^\top F^{\kappa_t})(q, p) \begin{pmatrix} -\iota \text{Id}_d \\ \text{Id}_d \end{pmatrix} \\ &\quad + \begin{pmatrix} \iota \text{Id}_d & \text{Id}_d \end{pmatrix} (F^{\kappa_t})^\top(q, p) \begin{pmatrix} 0 & -\iota \text{Id}_d \\ \iota \text{Id}_d & 0 \end{pmatrix} F^{\kappa_t}(q, p) \begin{pmatrix} -\iota \text{Id}_d \\ \text{Id}_d \end{pmatrix} \\ &= \begin{pmatrix} \iota \text{Id}_d & \text{Id}_d \end{pmatrix} ((F^{\kappa_t})^\top F^{\kappa_t})(q, p) \begin{pmatrix} -\iota \text{Id}_d \\ \text{Id}_d \end{pmatrix} + 2\text{Id}_d. \end{aligned}$$

In the last equality, we have used the property of symplecticity of  $F^{\kappa_t}(q, p)$ . Therefore  $(Z^{\kappa_t}(Z^{\kappa_t})^*)(q, p)$  is positive definite, which implies  $\det(Z^{\kappa_t}(q, p))$  is bounded away uniformly from zero for  $|p| > 0$ . The invertibility of  $Z^{\kappa_t}(q, p)$  and bounds (5.1) follows from the representation of  $(Z^{\kappa_t})^{-1}(q, p)$  by minors and Proposition 3.4.  $\square$

The following Lemma plays an important role in frozen Gaussian approximation.

**Lemma 5.2.** For each  $n = 1, \dots, N$ ,  $t \in [0, T]$ , let  $b(y, q, p) : \mathbb{R}^{3d} \rightarrow \mathbb{C}^N$  such that for any  $y \in \mathbb{R}^d$ ,  $\text{supp } b(y, \cdot, \cdot) \subset K_\delta$ . Assume that there exists some  $m \in \mathbb{R}$  that for any  $k \in \mathbb{N}$ ,

$$\sup_{y \in \mathbb{R}^d} (1 + |y|^2)^{-m/2} \Lambda_{k,\delta}[b(y, \cdot, \cdot)] < \infty.$$

Then for a multi-index  $(j_1, \dots, j_\nu)$  with  $\nu \geq 1$ ,

$$(5.2) \quad (x - Q_n(t, q, p))_{j_1} \cdots (x - Q_n(t, q, p))_{j_\nu} b(y, q, p) \sim \mathcal{T}_{n,j_1 \dots j_\nu}^{\nu, \varepsilon} b(y, q, p).$$

Here  $\mathcal{T}_{n,j_1 \dots j_\nu}^{\nu, \varepsilon}$  is defined by the recursive relation (4.6)-(4.8), corresponding to the  $n$ -th branch. Here, we have used the notation  $f \sim g$ , if

$$(5.3) \quad \int_{\mathbb{R}^{3d}} f(y, q, p) e^{\frac{\iota}{\varepsilon} \Phi_n(t, x, y, q, p)} dy dp dq = \int_{\mathbb{R}^{3d}} g(y, q, p) e^{\frac{\iota}{\varepsilon} \Phi_n(t, x, y, q, p)} dy dp dq.$$

*Proof.* We omit the subscript  $n$  in the proof for simplicity, because the argument is the same for each branch.

Observe that at  $t = 0$ , for  $|p| > 0$ ,

$$\begin{aligned}\partial_q S(0, q, p) - \partial_q Q(0, q, p)P(0, q, p) + p &= 0, \\ \partial_p S(0, q, p) - \partial_p Q(0, q, p)P(0, q, p) &= 0.\end{aligned}$$

Using (3.4) and (3.15), we have

$$\begin{aligned}\frac{d}{dt}(\partial_q S - \partial_q QP + p) &= \partial_q(\partial_t S) - \partial_q(\partial_t Q)P - \partial_q Q\partial_t P \\ &= \partial_q(P \cdot \partial_P H - H) - \partial_q(\partial_P H)P + \partial_q Q\partial_Q H \\ &= \partial_q P\partial_P H - (\partial_q Q\partial_Q + \partial_q P\partial_P)H + \partial_q Q\partial_Q H = 0,\end{aligned}$$

where  $S$ ,  $Q$  and  $P$  are evaluated at  $(t, q, p)$ , and  $\partial_Q H$ ,  $\partial_P H$  are evaluated at  $(Q, P)$ .

Analogously we have

$$\frac{d}{dt}(\partial_p S(t, q, p) - \partial_p Q(t, q, p)P(t, q, p)) = 0.$$

Therefore for all  $t \in [0, T]$ , we have

$$(5.4) \quad \partial_q S(t, q, p) - \partial_q Q(t, q, p)P(t, q, p) + p = 0,$$

$$(5.5) \quad \partial_p S(t, q, p) - \partial_p Q(t, q, p)P(t, q, p) = 0.$$

Straightforward calculations yield

$$\begin{aligned}\partial_q \Phi(t, x, y, q, p) &= (\partial_q P(t, q, p) - \imath \partial_q Q(t, q, p))(x - Q(t, q, p)) - \imath(y - q), \\ \partial_p \Phi(t, x, y, q, p) &= (\partial_p P(t, q, p) - \imath \partial_p Q(t, q, p))(x - Q(t, q, p)) - (y - q).\end{aligned}$$

This implies that

$$(5.6) \quad \imath \partial_z \Phi(t, x, y, q, p) = Z(t, q, p)(x - Q(t, q, p)),$$

where  $\partial_z$  and  $Z(t, q, p)$  are defined in (4.3).

Using (5.6) and Lemma 5.1 for the invertibility of  $Z(t, q, p)$  on the support of  $b(y, q, p)$ , one has, for  $j = 1, \dots, d$ ,

$$\begin{aligned}& \int_{\mathbb{R}^{3d}} (x - Q(t, q, p))_j e^{\frac{\imath}{\varepsilon} \Phi(t, x, y, q, p)} b(y, q, p) dy dq dp \\ &= \varepsilon \int_{\mathbb{R}^{3d}} Z_{jk}^{-1}(t, q, p) \left( \frac{\imath}{\varepsilon} \partial_{z_k} \Phi(t, x, y, q, p) \right) e^{\frac{\imath}{\varepsilon} \Phi(t, x, y, q, p)} b(y, q, p) dy dq dp.\end{aligned}$$

We remark that the integrability of the above integral follows from the exponential decay in  $y$  of  $\exp(\imath \Phi(t, x, y, q, p)/\varepsilon)$  and compact support of  $b(y, q, p)$  in  $(q, p)$ .



Integration by parts gives

$$\begin{aligned}
& \int_{\mathbb{R}^{3d}} (x - Q(t, q, p))_j e^{\frac{1}{\varepsilon} \Phi(t, x, y, q, p)} b(y, q, p) \, dy \, dq \, dp \\
&= -\varepsilon \int_{\mathbb{R}^{3d}} \partial_{z_k} (Z_{jk}^{-1}(t, q, p) b(y, q, p)) e^{\frac{1}{\varepsilon} \Phi(t, x, y, q, p)} \, dy \, dq \, dp \\
&= \int_{\mathbb{R}^{3d}} \varepsilon \mathcal{D}_j b(y, q, p) e^{\frac{1}{\varepsilon} \Phi(t, x, y, q, p)} \, dy \, dq \, dp \\
&= \int_{\mathbb{R}^{3d}} \mathcal{T}_j^{1, \varepsilon} b(y, q, p) e^{\frac{1}{\varepsilon} \Phi(t, x, y, q, p)} \, dy \, dq \, dp.
\end{aligned}$$

This proves (5.2) for  $\nu = 1$ .

Making use of the above equality twice produces (5.2) for  $\nu = 2$ ,

$$\begin{aligned}
& (x - Q(t, q, p))_{j_1} (x - Q(t, q, p))_{j_2} b(y, q, p) \\
&\quad \sim \varepsilon \mathcal{D}_{j_2} \left( (x - Q(t, q, p))_{j_1} b(y, q, p) \right) \\
&= \varepsilon \mathcal{G}_{j_1 j_2} b(y, q, p) + \varepsilon (x - Q(t, q, p))_{j_1} \mathcal{D}_{j_2} b(y, q, p) \\
&\quad \sim \varepsilon \mathcal{G}_{j_1 j_2} b(y, q, p) + \varepsilon^2 \mathcal{D}_{j_1} \mathcal{D}_{j_2} b(y, q, p) \\
&= \mathcal{T}_{j_1 j_2}^{2, \varepsilon} b(y, q, p).
\end{aligned}$$

Furthermore, we have

$$\begin{aligned}
& (x - Q(t, q, p))_{j_1} \cdots (x - Q(t, q, p))_{j_\nu} b(y, q, p) \\
&\quad \sim \varepsilon \mathcal{D}_{j_\nu} \left( (x - Q(t, q, p))_{j_1} \cdots (x - Q(t, q, p))_{j_{\nu-1}} b(y, q, p) \right) \\
&= \varepsilon (x - Q(t, q, p))_{j_1} \cdots (x - Q(t, q, p))_{j_{\nu-1}} \mathcal{D}_{j_\nu} b(y, q, p) \\
&\quad + \varepsilon \sum_{\alpha=1}^{\nu-1} (x - Q(t, q, p))_{j_1} \cdots (x - Q(t, q, p))_{j_{\alpha-1}} \\
&\quad \quad \times (x - Q(t, q, p))_{j_{\alpha+1}} \cdots (x - Q(t, q, p))_{j_{\nu-1}} \mathcal{G}_{j_\alpha j_\nu} b(y, q, p) \\
&\quad \sim \varepsilon \mathcal{T}_{j_1 j_2 \cdots j_{\nu-1}}^{\nu-1, \varepsilon} \mathcal{D}_{j_\nu} b(y, q, p) \\
&\quad + \varepsilon \sum_{\alpha=1}^{\nu-1} \mathcal{T}_{j_1 \cdots j_{\alpha-1} j_{\alpha+1} \cdots j_{\nu-1}}^{\nu-2, \varepsilon} \mathcal{G}_{j_\alpha j_\nu} b(y, q, p) \\
&= \mathcal{T}_{j_1 \cdots j_\nu}^{\nu, \varepsilon} b(y, q, p),
\end{aligned}$$

where the last step follows by the recursive relation (4.8). This proves (5.2) for  $\nu \geq 3$ . □

To construct a high order approximation to the solution, we need a filtered version of frozen Gaussian approximation, defined as follows. The relationship

between  $\tilde{\mathcal{P}}_{t,K,\delta}^\varepsilon$  and  $\mathcal{P}_{t,K,\delta}^\varepsilon$  will be addressed in Lemma 5.6 in the end of this section.

$$(5.7) \quad \begin{aligned} (\tilde{\mathcal{P}}_{t,K,\delta}^\varepsilon u_0)(x) &= \sum_{n=1}^N \left( \mathcal{I}_n^\varepsilon(t, \tilde{\mathcal{M}}_{n,K,t,\delta}^\varepsilon) u_0(y) \right) (x) \\ &= \frac{1}{(2\pi\varepsilon)^{3d/2}} \sum_{n=1}^N \int_{\mathbb{R}^{3d}} e^{i\Phi_n(t,x,y,q,p)/\varepsilon} \tilde{\mathcal{M}}_{n,K,t,\delta}^\varepsilon(q,p) u_0(y) \, dq \, dp \, dy. \end{aligned}$$

Here the matrix-valued function  $\tilde{\mathcal{M}}_{n,K,t,\delta}^\varepsilon : \mathbb{R}^{2d} \rightarrow \mathbb{C}^{N \times N}$  is given by

$$(5.8) \quad \tilde{\mathcal{M}}_{n,K,t,\delta}^\varepsilon(q,p) = \tilde{\mathcal{M}}_{n,K,\delta}^\varepsilon(t,q,p) = \sum_{k=0}^{K-1} \varepsilon^k \tilde{M}_{n,k,\delta}(t,q,p).$$

For  $(q,p) \in \mathbb{R}^{2d}$  and  $t \in [0, T]$ ,  $\tilde{M}_{n,k,\delta}(t,q,p)$  is defined as follows. For  $k=0$ ,

$$(5.9) \quad \tilde{M}_{n,0,\delta}(t,q,p) = \tilde{\sigma}_{n,0,\delta}(t,q,p) R_n(Q_n(t,q,p), P_n(t,q,p)) L_n^\top(q,p) \chi_\delta(q,p),$$

where  $\chi_\delta(q,p)$  is the filter function given before, and  $\tilde{\sigma}_{n,0,\delta}(t,q,p)$  satisfies

$$(5.10) \quad \frac{d}{dt} \tilde{\sigma}_{n,0,\delta}(t,q,p) \chi_\delta(q,p) + \tilde{\sigma}_{n,0,\delta}(t,q,p) \lambda_n(t,q,p) \chi_\delta(q,p) = 0,$$

with the initial condition  $\tilde{\sigma}_{n,0,\delta}(0,q,p) = 2^{d/2}$  and  $\lambda_n(t,q,p)$  is given by (4.16).

For  $k \geq 1$ ,  $\tilde{M}_{n,k,\delta}$  is given recursively by

$$(5.11) \quad \tilde{M}_{n,k,\delta}(t,q,p) = \tilde{\sigma}_{n,k,\delta}(t,q,p) R_n(Q_n, P_n) L_n(q,p)^\top \chi_\delta(q,p) + \tilde{M}_{n,k,\delta}^\perp(t,q,p),$$

where  $\tilde{M}_{n,k,\delta}^\perp(t,q,p)$  is given by

$$(5.12) \quad \tilde{M}_{n,k,\delta}^\perp(t,q,p) = \mathcal{L}_{n,0}^\dagger(Q_n, P_n) \sum_{s=1}^k (\mathcal{L}_{n,s} \tilde{M}_{n,k-s,\delta})(t,q,p),$$

and  $\tilde{\sigma}_{n,k,\delta}(t,q,p)$  satisfies

$$(5.13) \quad \begin{aligned} \frac{d}{dt} \tilde{\sigma}_{n,k,\delta}(t,q,p) \chi_\delta(q,p) + \tilde{\sigma}_{n,k,\delta}(t,q,p) \lambda_n(t,q,p) \chi_\delta(q,p) \\ + L_n(Q_n, P_n)^\top \left( (\mathcal{L}_{n,1} \tilde{M}_{n,k,\delta}^\perp)(t,q,p) \right. \\ \left. + \sum_{s=2}^{k+1} (\mathcal{L}_{n,s} \tilde{M}_{n,k+1-s,\delta})(t,q,p) \right) R_n(q,p) = 0, \end{aligned}$$

with the initial condition  $\tilde{\sigma}_{n,k,\delta}(0,q,p) = 0$ . In (5.12) and (5.13),  $Q_n$  and  $P_n$  are evaluated at  $(t,q,p)$ . We remark that, from the definitions (5.9) and (5.11), it is clear that the value of  $\tilde{\sigma}_{n,k,\delta}(t,q,p)$  outside  $\text{supp } \chi_\delta(q,p) \subset K_{\delta/2}$  will not affect the value of  $\tilde{M}_{n,k,\delta}(t,q,p)$ .

**Lemma 5.3.** *For each  $n = 1, \dots, N$ ,  $k \in \mathbb{N}$  and any  $\delta > 0$ , there exists constant  $C_{k,\delta}$  that*

$$(5.14) \quad \Lambda_{k,\delta}[\mathcal{L}_{n,0}^\dagger(q,p)] \leq C_{k,\delta}.$$

*Proof.* Recall that  $\mathcal{L}_{n,0}^\dagger(q,p)$  is defined in (4.17) as

$$\mathcal{L}_{n,0}^\dagger(q,p) = \iota \sum_{m \neq n} (H_n(q,p) - H_m(q,p))^{-1} R_m(q,p) L_m^\top(q,p).$$

By strict hyperbolicity and compactness, there exists  $g_\delta > 0$  such that

$$(5.15) \quad \inf_{(q,p) \in K_\delta} \inf_{n \neq m} |H_n(q,p) - H_m(q,p)| \geq g_\delta.$$

The estimate (5.14) follows easily.  $\square$

**Lemma 5.4.** *For each  $n = 1, \dots, N$ , any  $t \in [0, T]$  and any  $k \in \mathbb{N}$ , we have  $\text{supp } \widetilde{M}_{n,k,\delta}(t, \cdot, \cdot) \subset K_{\delta/2}$ ,  $\text{supp } \partial_t \widetilde{M}_{n,k,\delta}(t, \cdot, \cdot) \subset K_{\delta/2}$ . Moreover, for any  $s \in \mathbb{N}$ , there exists constant  $C_{k,s,\delta,T}$  that*

$$\begin{aligned} \sup_{t \in [0, T]} \Lambda_{s,\delta/2}[\widetilde{M}_{n,k,\delta}(t, q, p)] &\leq C_{k,s,\delta,T}; \\ \sup_{t \in [0, T]} \Lambda_{s,\delta/2}[\partial_t \widetilde{M}_{n,k,\delta}(t, q, p)] &\leq C_{k,s,\delta,T}. \end{aligned}$$

*Proof.* The argument is the same for each branch, so we will omit the subscript  $n$  in the proof.

By Proposition 3.1, there exists constant  $\delta_T$  such that for  $t \in [0, T]$ , we have  $(Q(t, q, p), P(t, q, p)) \in K_{\delta_T}$  for  $(q, p) \in K_{\delta/2}$ . From Lemma 5.1 and Proposition 3.2, it is easy to conclude that for any  $s \in \mathbb{N}$  and  $l = 0, 1$ ,

$$(5.16) \quad \sup_{t \in [0, T]} \Lambda_{s,\delta/2}[\partial_t^l \lambda(t, q, p)] \leq C_{s,\delta,T}.$$

Equation (5.9) implies that

$$\text{supp } \widetilde{M}_{0,\delta}(t, q, p) \subset \text{supp } \chi_\delta(q, p) \subset K_{\delta/2}.$$

Moreover, (5.10) implies that

$$\frac{d}{dt} |\widetilde{\sigma}_{0,\delta}(t, q, p) \chi_\delta(q, p)| \leq |\lambda(t, q, p)| |\widetilde{\sigma}_{0,\delta}(t, q, p) \chi_\delta(q, p)|.$$

Hence Gronwall's inequality yields

$$\sup_{t \in [0, T]} \sup_{(q,p) \in K_{\delta/2}} |\widetilde{\sigma}_{0,\delta}(t, q, p) \chi_\delta(q, p)| \leq C_{\delta,T}.$$

Taking derivatives of (5.10) with respect to  $(t, q, p)$ , we have for multi-index  $\alpha$  and  $l = 0, 1$ ,

$$\begin{aligned} &\frac{d}{dt} \partial_{(q,p)}^\alpha \partial_t^l (\widetilde{\sigma}_{0,\delta}(t, q, p) \chi_\delta(q, p)) \\ &= \sum_{\beta \leq \alpha} \sum_{0 \leq m \leq l} \binom{\alpha}{\beta} \partial_{(q,p)}^\beta \partial_t^m \lambda(t, q, p) \partial_{(q,p)}^{\alpha-\beta} \partial_t^{l-m} (\widetilde{\sigma}_{0,\delta}(t, q, p) \chi_\delta(q, p)). \end{aligned}$$

Using (5.16) and by induction, we have for  $l = 0, 1$ ,

$$\sup_{t \in [0, T]} \Lambda_{s, \delta/2} [\partial_t^l (\tilde{\sigma}_{0, \delta}(t, q, p) \chi_\delta(q, p))] \leq C_{s, \delta, T},$$

which implies

$$(5.17) \quad \sup_{t \in [0, T]} \Lambda_{s, \delta/2} [\partial_t^l \tilde{M}_{0, \delta}(t, q, p)] \leq C_{s, \delta, T}.$$

Next, we consider  $\tilde{M}_{1, \delta}(t, q, p)$ . (5.12) gives

$$\tilde{M}_{1, \delta}^\perp(t, q, p) = \mathcal{L}_0^\dagger(Q_n(t, q, p), P_n(t, q, p))(\mathcal{L}_1 \tilde{M}_{0, \delta})(t, q, p).$$

As  $\text{supp } \tilde{M}_{0, \delta}(t, q, p) \subset K_{\delta/2}$ , we have  $\text{supp } \tilde{M}_{1, \delta}^\perp(t, q, p) \subset K_{\delta/2}$ . By Lemma 5.3, (4.11) and (5.17), it is not hard to see that for  $l = 0, 1$ ,

$$\sup_{t \in [0, T]} \Lambda_{s, \delta/2} [\partial_t^l \tilde{M}_{1, \delta}^\perp(t, q, p)] \leq C_{s, \delta, T}.$$

Similarly, we get from (5.13) the estimate

$$\sup_{t \in [0, T]} \Lambda_{s, \delta/2} [\partial_t^l \tilde{\sigma}_{1, \delta}(t, q, p) \chi_\delta(q, p)] \leq C_{s, \delta, T}.$$

In summary, we obtain  $\text{supp } \tilde{M}_{1, \delta}(t, q, p) \subset K_{\delta/2}$ , and for  $l = 0, 1$ ,

$$\sup_{t \in [0, T]} \Lambda_{s, \delta/2} [\partial_t^l \tilde{M}_{1, \delta}(t, q, p)] \leq C_{s, \delta, T}.$$

Continuing this procedure, we obtain the estimates for higher order asymptotic terms:  $\text{supp } \tilde{M}_{k, \delta}(t, q, p) \subset \text{supp } K_{\delta/2}$  for  $k \geq 0$ , and

$$\begin{aligned} \sup_{t \in [0, T]} \Lambda_{s, \delta/2} [\tilde{M}_{k, \delta}(t, q, p)] &\leq C_{k, s, \delta, T}, \\ \sup_{t \in [0, T]} \Lambda_{s, \delta/2} [\partial_t \tilde{M}_{k, \delta}(t, q, p)] &\leq C_{k, s, \delta, T}. \end{aligned}$$

This proves the Lemma. □

We now show that the filtered frozen Gaussian approximation gives a high order approximation to the solution.

**Proposition 5.5.** *Under the same assumption of Theorem 4.1, for any  $T > 0$ ,  $K \in \mathbb{N}$ , there exists constant  $C_{T, K}$ , so that for any  $\varepsilon > 0$ ,*

$$\left\| (\partial_t + A_t(x) \partial_{x_l}) \tilde{\mathcal{P}}_{t, K, \delta}^\varepsilon u_0^\varepsilon \right\|_{L^2(\mathbb{R}^d)} \leq C_{T, K} M \varepsilon^{K-1}.$$

*Proof.* Without further indication,  $S_n$ ,  $Q_n$  and  $P_n$  are all evaluated at  $(t, q, p)$  in the proof.

For each  $l = 1, \dots, d$ , Taylor expansion of  $A_l(x)$  around  $x = Q_n$  gives

$$(5.18) \quad A_l(x) = A_l(Q_n) + \sum_{\nu=1}^{2K} \frac{1}{\nu!} (x - Q_n)_{j_1} \cdots (x - Q_n)_{j_\nu} \partial_{j_1 \dots j_\nu}^\nu A_l(Q_n) \\ + \frac{1}{(2K)!} (x - Q_n)_{j_1} \cdots (x - Q_n)_{j_{2K+1}} \widehat{A}_{l, j_1 \dots j_{2K+1}}(Q_n),$$

where  $\widehat{A}_{l, j_1 \dots j_{2K+1}}(Q_n)$  is the integral

$$(5.19) \quad \widehat{A}_{l, j_1 \dots j_{2K+1}}(Q_n) = \int_0^1 (1 - \tau)^{2K} \partial_{j_1 \dots j_{2K+1}}^{2K+1} A_l(Q_n + \tau(x - Q_n)) \, d\tau.$$

We define the operators  $\widetilde{\mathcal{L}}_{n,k}$  on  $C^1([0, T], C^\infty(\mathbb{R}^{2d}; \mathbb{C}^{N \times N}))$  as follows. For  $M : \mathbb{R} \times \mathbb{R}^{2d} \rightarrow \mathbb{C}^{N \times N}$ , we define for  $0 \leq k \leq K$ ,

$$(\widetilde{\mathcal{L}}_{n,k} M)(t, q, p) = (\mathcal{L}_{n,k} M)(t, q, p),$$

for  $K + 1 \leq k \leq 2K + 2$ ,

$$(\widetilde{\mathcal{L}}_{n,k} M)(t, q, p) = \sum_{\nu=k}^{2K} \mathcal{T}_{n, j_1 \dots j_\nu}^{\nu, k} \left( \left( -\frac{1}{(\nu-1)!} \partial_{j_1 \dots j_{\nu-1}}^{\nu-1} A_{j_\nu}(Q_n) \right. \right. \\ \left. \left. + \frac{i}{\nu!} P_l \partial_{j_1 \dots j_\nu}^\nu A_l(Q_n) \right) M(t, q, p) \right) \\ + \mathcal{T}_{n, j_1 \dots j_{2K+1}}^{2K+1, k} \left( \left( -\frac{1}{(2K)!} \partial_{j_1 \dots j_{2K}}^{2K} A_{j_{2K+1}}(Q_n) \right. \right. \\ \left. \left. + \frac{i}{(2K)!} P_l \widehat{A}_{l, j_1 \dots j_{2K+1}}(Q_n) \right) M(t, q, p) \right) \\ + \mathcal{T}_{n, j_1 \dots j_{2K+2}}^{2K+2, k} \left( -\frac{1}{(2K)!} \widehat{A}_{j_{2K+2}, j_1 \dots j_{2K+1}}(Q_n) M(t, q, p) \right),$$

and for  $k \geq 2K + 3$ ,

$$(\widetilde{\mathcal{L}}_{n,k} M)(t, q, p) = 0.$$

Differentiating  $\Phi_n(t, x, y, q, p)$  with respect to  $t$  and  $x$  gives

$$\partial_t \Phi_n(t, x, y, q, p) = \partial_t S_n - P_n \cdot \partial_t Q_n + (x - Q_n) \cdot (\partial_t P_n - i \partial_t Q_n), \\ \partial_x \Phi_n(t, x, y, q, p) = i(x - Q_n) + P_n.$$

Combining these expressions, substituting (5.7) and (5.18) into (3.1), and organizing terms in orders of  $\varepsilon$  produce, after straightforward calculations,

$$(\partial_t + A_l(x) \partial_{x_l}) (\widetilde{\mathcal{P}}_{t, K, \delta}^\varepsilon u_0^\varepsilon)(x) = \sum_{k=0}^{K-1} \varepsilon^{k-1} v_{t, k, \delta}(x) + \varepsilon^{K-1} r_{t, K, \delta}(x),$$

where we have,

$$\begin{aligned}
v_{t,0,\delta}(x) &= \sum_{n=1}^N (2\pi\varepsilon)^{-3d/2} \int_{\mathbb{R}^{3d}} (\tilde{\mathcal{L}}_{n,0} \tilde{M}_{n,0,\delta})(t, q, p) e^{i\Phi_n/\varepsilon} u_0^\varepsilon(y) \, dy \, dp \, dq, \\
v_{t,1,\delta}(x) &= \sum_{n=1}^N (2\pi\varepsilon)^{-3d/2} \int_{\mathbb{R}^{3d}} ((\tilde{\mathcal{L}}_{n,0} \tilde{M}_{n,1,\delta})(t, q, p) \\
&\quad + (\tilde{\mathcal{L}}_{n,1} \tilde{M}_{n,0,\delta})(t, q, p)) e^{i\Phi_n/\varepsilon} u_0^\varepsilon(y) \, dy \, dp \, dq, \\
v_{t,k,\delta}(x) &= \sum_{n=1}^N (2\pi\varepsilon)^{-3d/2} \int_{\mathbb{R}^{3d}} \sum_{s=0}^k (\tilde{\mathcal{L}}_{n,s} \tilde{M}_{n,k-s,\delta})(t, q, p) e^{i\Phi_n/\varepsilon} u_0^\varepsilon(y) \, dy \, dp \, dq,
\end{aligned}$$

and the remainder,

$$\begin{aligned}
r_{t,K,\delta}(x) &= \sum_{k=0}^{2K+1} \varepsilon^k \sum_{s=0}^{K-1} \sum_{n=1}^N (2\pi\varepsilon)^{-3d/2} \\
&\quad \times \int_{\mathbb{R}^{3d}} (\tilde{\mathcal{L}}_{n,k+s+1} \tilde{M}_{n,K-s-1,\delta})(t, q, p) e^{i\Phi_n/\varepsilon} u_0^\varepsilon(y) \, dy \, dp \, dq.
\end{aligned}$$

Here  $\Phi_n$  is evaluated at  $(t, x, y, q, p)$ .

We will show that  $v_{t,k,\delta} = 0$  for  $k = 0, \dots, K-1$  and control the norm of the remainder  $r_{t,K,\delta}$  to prove the proposition.

By definitions of  $R_n(Q_n, P_n)$  as in (3.3) and of  $S_n$  as in (3.15), we get

$$\begin{aligned}
& \left( \partial_t S_n - P_n \cdot \partial_t Q_n + P_{n,l} A_l(Q_n) \right) R_n(Q_n, P_n) \\
&= \left( \partial_t S_n - P_n \cdot \partial_t Q_n + H_n(Q_n, P_n) \right) R_n(Q_n, P_n) = 0,
\end{aligned}$$

which implies  $(\tilde{\mathcal{L}}_{n,0} \tilde{M}_{n,0,\delta})(t, q, p) = 0$  for each  $n$ , since  $\tilde{M}_{n,0,\delta}$  is given as (5.9). Therefore,  $v_{t,0,\delta} = 0$ .

To prove  $v_{t,1,\delta} = 0$ , it suffices to show that, for each  $m = 1, \dots, N$ ,

$$(5.20) \quad L_m^\top(Q_n, P_n) \left( (\tilde{\mathcal{L}}_{n,0} \tilde{M}_{n,1,\delta})(t, q, p) + (\tilde{\mathcal{L}}_{n,1} \tilde{M}_{n,0,\delta})(t, q, p) \right) = 0.$$

When  $m \neq n$ , (5.20) is equivalent to, by (3.3),

$$(5.21) \quad L_m^\top(Q_n, P_n) \left( (\tilde{\mathcal{L}}_{n,0} \tilde{M}_{n,1,\delta}^\perp)(t, q, p) + (\tilde{\mathcal{L}}_{n,1} \tilde{M}_{n,0,\delta})(t, q, p) \right) = 0,$$

which is valid by (4.17) and (5.12).

When  $m = n$ , (5.20) is equivalent to, by (3.2),

$$(5.22) \quad L_n^\top(Q_n, P_n) (\tilde{\mathcal{L}}_{n,1} \tilde{M}_{n,0,\delta})(t, q, p) = 0,$$

which will be proved as follows. For convenience, we will omit the index  $n$  in the following calculations. Substituting (5.9) in (5.22) and using (4.4), (4.5) and (4.11),

we can rewrite (5.22) as

$$\begin{aligned}
(5.23) \quad & L^T(Q, P) \left( \partial_t(\tilde{\sigma}_{0,\delta}(t, q, p)R(Q, P))L^T(q, p)\chi_\delta(q, p) \right. \\
& \quad - \partial_{z_k} \left( (\imath\partial_t P_j + \partial_t Q_j - A_j(Q) + \imath P_l \partial_j A_l(Q)) \right. \\
& \quad \quad \left. \left. \times \tilde{\sigma}_{0,\delta}(t, q, p)R(Q, P)Z_{jk}^{-1}L^T(q, p)\chi_\delta(q, p) \right) \right. \\
& \quad \left. + \partial_{z_s} Q_j \left( -\partial_j A_k(Q) + \frac{\imath}{2} P_l \partial_{jk}^2 A_l(Q) \right) \right. \\
& \quad \quad \left. \left. \times \tilde{\sigma}_{0,\delta}(t, q, p)R(Q, P)Z_{ks}^{-1}L^T(q, p)\chi_\delta(q, p) \right) \right) = 0.
\end{aligned}$$

For the first term, easy calculations yield

$$\begin{aligned}
& L^T(Q, P) \left( \partial_t(\tilde{\sigma}_{0,\delta}(t, q, p)R(Q, P))L^T(q, p)\chi_\delta(q, p) \right) \\
& = \left( \partial_t \tilde{\sigma}_{0,\delta}(t, q, p) + \tilde{\sigma}_{0,\delta}(t, q, p)L^T(Q, P) \left( \partial_P H(Q, P) \cdot \partial_Q R(Q, P) \right. \right. \\
& \quad \left. \left. - \partial_Q H(Q, P) \cdot \partial_P R(Q, P) \right) \right) L^T(q, p)\chi_\delta(q, p).
\end{aligned}$$

To simplify the second term in (5.23), we observe that differentiating (3.3) with respect to  $P$  and  $Q$  yields,

$$\begin{aligned}
& A_l(Q)R(Q, P) + P_j A_j(Q)\partial_{P_l} R(Q, P) \\
& = \partial_{P_l} H(Q, P)R(Q, P) + H(Q, P)\partial_{P_l} R(Q, P),
\end{aligned}$$

and

$$\begin{aligned}
& P_j \partial_l A_j(Q)R(Q, P) + P_j A_j(Q)\partial_{Q_l} R(Q, P) \\
& = \partial_{Q_l} H(Q, P)R(Q, P) + H(Q, P)\partial_{Q_l} R(Q, P).
\end{aligned}$$

Taking inner product with  $L(Q, P)$  on the left produces

$$(5.24) \quad L^T(Q, P)(A_l(Q) - \partial_{P_l} H(Q, P))R(Q, P) = 0,$$

$$(5.25) \quad L^T(Q, P)(P_j \partial_l A_j(Q) - \partial_{Q_l} H(Q, P))R(Q, P) = 0.$$

Define the short hand notation

$$\begin{aligned}
F_j(t, q, p) &= (\imath\partial_t P_j + \partial_t Q_j)R(Q, P) - A_j(Q)R(Q, P) + \imath P_l \partial_j A_l(Q)R(Q, P) \\
&= - \left( (A_j(Q) - \partial_{P_j} H(Q, P)) + \imath(\partial_{Q_j} H(Q, P) - P_l \partial_j A_l(Q)) \right) R(Q, P).
\end{aligned}$$

Using (5.24) and (5.25), it is clear that for any  $j = 1, \dots, d$ ,

$$L^T(Q, P)F_j(t, q, p) = 0.$$

Hence,

$$\begin{aligned}
& L^T(Q, P)\partial_{z_k} \left( (\tilde{\sigma}_{0,\delta} F_j Z_{jk}^{-1})(t, q, p)L^T(q, p)\chi_\delta(q, p) \right) \\
& = \tilde{\sigma}_{0,\delta}(t, q, p)L^T(Q, P)(\partial_{z_k} F_j Z_{jk}^{-1})(t, q, p)L^T(q, p)\chi_\delta(q, p) \\
& = -\tilde{\sigma}_{0,\delta}(t, q, p)(\partial_{z_k} L)^T(Q, P)(F_j Z_{jk}^{-1})(t, q, p)L^T(q, p)\chi_\delta(q, p).
\end{aligned}$$

Therefore, (5.23) is implied by

$$\begin{aligned} & \partial_t \tilde{\sigma}_{0,\delta}(t, q, p) \chi_\delta(q, p) + \tilde{\sigma}_{0,\delta}(t, q, p) L^\top (\partial_P H \cdot \partial_Q R - \partial_Q H \cdot \partial_P R) \chi_\delta(q, p) \\ & + \tilde{\sigma}_{0,\delta}(t, q, p) (\partial_{z_k} L)^\top (F_j Z_{jk}^{-1})(t, q, p) \chi_\delta(q, p) \\ & + \tilde{\sigma}_{0,\delta}(t, q, p) \partial_{z_s} Q_j Z_{ks}^{-1}(t, q, p) \\ & \quad \times L^\top (-\partial_j A_k(Q) + \frac{i}{2} P_l \partial_{jk}^2 A_l(Q)) \chi_\delta(q, p) = 0, \end{aligned}$$

which is valid by (5.10) and (4.16). Here in the last equation,  $H$ ,  $L$  and  $R$  are evaluated at  $(Q, P)$ .

Similarly, we can show that  $v_{t,k,\delta}(x) = 0$  for higher orders, by using (5.11)-(5.13).

Therefore, to prove the Lemma, it remains to bound the remainder  $r_{t,K,\delta}(x)$ . Using Proposition 3.7, it suffices to control the  $L^\infty$  norm of  $(\tilde{L}_{n,k} \tilde{M}_{n,s,\delta})(t, q, p)$  for  $k = 1, \dots, 2K+2$  and  $s = 0, \dots, K-1$ . This in turn follows from Lemma 5.4 and the definition of  $\tilde{L}_{n,k}$ .  $\square$

To relate  $\tilde{\mathcal{P}}_{t,K,\delta}^\varepsilon$  with  $\mathcal{P}_{t,K,\delta}^\varepsilon$  defined in (4.1), the following lemma shows that they are essentially the same when applying on asymptotically high frequency initial data.

**Lemma 5.6.** *For any  $T > 0$ ,  $K \in \mathbb{N}$ ,*

$$\sup_{0 \leq t \leq T} \left\| \mathcal{P}_{t,K,\delta}^\varepsilon u_0^\varepsilon - \tilde{\mathcal{P}}_{t,K,\delta}^\varepsilon u_0^\varepsilon \right\|_{L^2(\mathbb{R}^d; \mathbb{C}^N)} = \mathcal{O}(\varepsilon^\infty).$$

*Proof.* By definition (4.1) and (5.7),

$$\begin{aligned} (\mathcal{P}_{t,K,\delta}^\varepsilon u_0^\varepsilon - \tilde{\mathcal{P}}_{t,K,\delta}^\varepsilon u_0^\varepsilon)(x) &= \frac{1}{(2\pi\varepsilon)^{3d/2}} \sum_{n=1}^N \sum_{k=0}^{K-1} \int_{\mathbb{R}^{3d}} e^{i\Phi_n/\varepsilon} \\ & \quad \times \varepsilon^k \left( M_{n,k}(t, q, p) \chi_\delta(q, p) - \tilde{M}_{n,k,\delta}(t, q, p) \right) u_0(y) \, dq \, dp \, dy. \end{aligned}$$

From the constructions of  $M_{n,k}$  and  $\tilde{M}_{n,k,\delta}$ , it is easy to see that for  $t \in [0, T]$  and  $(q, p) \in K_\delta$ .

$$(5.26) \quad M_{n,k}(t, q, p) = \tilde{M}_{n,k,\delta}(t, q, p).$$

As  $\chi_\delta(q, p) = 1$  for  $(q, p) \in K_\delta$ , we have

$$M_{n,k}(t, q, p) \chi_\delta(q, p) = \tilde{M}_{n,k,\delta}(t, q, p).$$

Using (5.26) with  $\delta/2$ , we have then

$$(5.27) \quad M_{n,k}(t, q, p) = \tilde{M}_{n,k,\delta/2}(t, q, p)$$

for  $(q, p) \in K_{\delta/2}$ , and hence in particular, for  $(q, p) \in \text{supp } \chi_\delta$ . Combining (5.27) with Lemma 5.4 gives

$$(5.28) \quad \sup_{t \in [0, T]} \sup_{(q, p) \in \mathbb{R}^{2d}} |M_{n,k}(t, q, p) \chi_\delta(q, p)| \leq C_T.$$



Lemma 5.4 guarantees  $\text{supp } \widetilde{M}_{n,k,\delta}(t, \cdot, \cdot) \subset K_{\delta/2}$ . Since  $\text{supp } \chi_\delta \subset K_{\delta/2}$ , we also have  $\text{supp}(M_{n,k}(t, \cdot, \cdot)\chi_\delta) \subset K_{\delta/2}$ . Therefore, by (5.26), we have

$$(5.29) \quad \text{supp}\left(M_{n,k}(t, \cdot, \cdot)\chi_\delta - \widetilde{M}_{n,k,\delta}(t, \cdot, \cdot)\right) \subset K_{\delta/2} \setminus K_\delta.$$

Using a similar argument as in the proof of Proposition 3.7, one has

$$\begin{aligned} & \left\| \mathcal{P}_{t,K,\delta}^\varepsilon u_0^\varepsilon - \widetilde{\mathcal{P}}_{t,K,\delta}^\varepsilon u_0^\varepsilon \right\|_{L^2(\mathbb{R}^d; \mathbb{C}^N)} \\ & \leq 2^{-d/2} \sum_{n=1}^N \sum_{k=0}^{K-1} \varepsilon^k \left\| (M_{n,k}(t, \cdot, \cdot)\chi_\delta - \widetilde{M}_{n,k,\delta}(t, \cdot, \cdot)) \mathcal{F}^\varepsilon u_0^\varepsilon \right\|_{L^2(\mathbb{R}^{2d}; \mathbb{C}^N)} \\ & \leq 2^{-d/2} \sum_{n=1}^N \sum_{k=0}^{K-1} \varepsilon^k \left\| (M_{n,k}(t, \cdot, \cdot)\chi_\delta - \widetilde{M}_{n,k,\delta}(t, \cdot, \cdot)) \right\|_{L^\infty(\mathbb{R}^{2d}; \mathbb{C}^{N \times N})} \\ & \quad \times \left\| \mathcal{F}^\varepsilon u_0^\varepsilon \right\|_{L^2(K_{\delta/2} \setminus K_\delta; \mathbb{C}^N)} \\ & \leq C_{\delta,T,K} \left\| \mathcal{F}^\varepsilon u_0^\varepsilon \right\|_{L^2(K_{\delta/2} \setminus K_\delta; \mathbb{C}^N)}, \end{aligned}$$

where we have used (5.29) in the second inequality, and (5.28) and Lemma 5.4 in the last inequality. The proof is concluded by noticing that

$$\left\| \mathcal{F}^\varepsilon u_0^\varepsilon \right\|_{L^2(K_{\delta/2} \setminus K_\delta; \mathbb{C}^N)} \leq \left\| \mathcal{F}^\varepsilon u_0^\varepsilon \right\|_{L^2(\mathbb{R}^{2d} \setminus K_\delta; \mathbb{C}^N)} = \mathcal{O}(\varepsilon^\infty),$$

by Definition 2.2.  $\square$

## 6. PROOF OF THE MAIN RESULTS

We recall the energy estimate for linear strictly hyperbolic system. The proof can be found for example in [21].

**Lemma 6.1.** *Given strictly hyperbolic system*

$$\partial_t u + \sum_{l=1}^d A_l(x) \partial_{x_l} u = f,$$

with initial condition  $u(0, x) = u_0(x)$ , where  $A_l(x)$  are given as in (3.1). For any  $T > 0$ , there exists a constant  $C_T$  such that

$$\sup_{0 \leq t \leq T} \|u(t, x)\|_{L^2(\mathbb{R}^d; \mathbb{C}^N)}^2 \leq C_T \left( \|u_0(x)\|_{L^2(\mathbb{R}^d; \mathbb{C}^N)}^2 + \int_0^T \|f(s, x)\|_{L^2(\mathbb{R}^d; \mathbb{C}^N)}^2 ds \right).$$

**Proposition 6.2.** *Under the same assumption of Theorem 4.1, for any  $K \in \mathbb{N}$ ,  $T > 0$ , there exists constants  $C_{T,K}$  and  $\varepsilon_0 > 0$ , such that for any  $\varepsilon \in (0, \varepsilon_0]$ ,*

$$(6.1) \quad \sup_{t \in [0, T]} \left\| \mathcal{P}_t u_0^\varepsilon - \widetilde{\mathcal{P}}_{t,K,\delta}^\varepsilon u_0^\varepsilon \right\|_{L^2(\mathbb{R}^d; \mathbb{C}^N)} \leq C_{T,K} M \varepsilon^{K-1}.$$

*Proof.* We denote

$$e^\varepsilon(t, x) = (\mathcal{P}_t u_0^\varepsilon)(x) - (\widetilde{\mathcal{P}}_{t,K,\delta}^\varepsilon u_0^\varepsilon)(x).$$

Proposition 5.5 implies

$$\sup_{t \in [0, T]} \|(\partial_t + A_l(x) \partial_{x_l}) e^\varepsilon(t, \cdot)\|_{L^2(\mathbb{R}^d; \mathbb{C}^N)} \leq C_{T,K} M \varepsilon^{K-1}.$$

Notice that by the construction of filtered frozen Gaussian approximation,

$$\begin{aligned} (\tilde{\mathcal{P}}_{0,K,\delta}^\varepsilon u_0^\varepsilon)(x) &= \frac{1}{(2\pi\varepsilon)^{3d/2}} \sum_{n=1}^N \int_{\mathbb{R}^{3d}} e^{-|x-q|^2/(2\varepsilon)+ip\cdot(x-q)/\varepsilon-|y-q|^2/(2\varepsilon)-ip\cdot(y-q)/\varepsilon} \\ &\quad \times 2^{d/2} R_n(q,p) L_n^\top(q,p) \chi_\delta(q,p) u_0^\varepsilon(y) dq dp dy \\ &= (\mathcal{F}^\varepsilon)^*(\chi_\delta \mathcal{F}^\varepsilon u_0^\varepsilon), \end{aligned}$$

where we have used that fact that for  $(q,p) \in \mathbb{R}^{2d}$  with  $|p| > 0$ ,

$$\sum_{n=1}^N R_n(q,p) L_n^\top(q,p) = \text{Id}_N.$$

This implies

$$e^\varepsilon(0,x) = u_0^\varepsilon(x) - (\tilde{\mathcal{P}}_{0,K,\delta}^\varepsilon u_0^\varepsilon)(x) = (\mathcal{F}^\varepsilon)^*((1-\chi_\delta)\mathcal{F}^\varepsilon u_0^\varepsilon).$$

Hence, using Proposition 2.1,

$$\|e^\varepsilon(0,\cdot)\|_{L^2(\mathbb{R}^d;\mathbb{C}^N)} = \|(1-\chi_\delta)\mathcal{F}^\varepsilon u_0^\varepsilon\|_{L^2(\mathbb{R}^{2d};\mathbb{C}^N)} \leq \|\mathcal{F}^\varepsilon u_0^\varepsilon\|_{L^2(\mathbb{R}^{2d}\setminus K_\delta;\mathbb{C}^N)} = \mathcal{O}(\varepsilon^\infty).$$

The conclusion of the Proposition follows easily from Lemma 6.1.  $\square$

Finally, we conclude with the proof of Theorem 4.1.

*Proof of Theorem 4.1.* Triangle inequality gives

$$\begin{aligned} \|\mathcal{P}_t u_0^\varepsilon - \mathcal{P}_{t,K,\delta}^\varepsilon u_0^\varepsilon\|_{L^2(\mathbb{R}^d;\mathbb{C}^N)} &\leq \|\mathcal{P}_t u_0^\varepsilon - \tilde{\mathcal{P}}_{t,K+1,\delta}^\varepsilon u_0^\varepsilon\|_{L^2(\mathbb{R}^d;\mathbb{C}^N)} \\ &\quad + \|\tilde{\mathcal{P}}_{t,K+1,\delta}^\varepsilon u_0^\varepsilon - \mathcal{P}_{t,K+1,\delta}^\varepsilon u_0^\varepsilon\|_{L^2(\mathbb{R}^d;\mathbb{C}^N)} \\ &\quad + \|\mathcal{P}_{t,K+1,\delta}^\varepsilon u_0^\varepsilon - \mathcal{P}_{t,K,\delta}^\varepsilon u_0^\varepsilon\|_{L^2(\mathbb{R}^d;\mathbb{C}^N)}. \end{aligned}$$

The first two terms are estimated by Lemma 5.6 and Proposition 6.2. For the last term, notice that by definition

$$\mathcal{P}_{t,K+1,\delta}^\varepsilon u_0^\varepsilon - \mathcal{P}_{t,K,\delta}^\varepsilon u_0^\varepsilon = \mathcal{I}_n^\varepsilon(t, \varepsilon^K M_{n,K}(t, \cdot, \cdot) \chi_\delta) u_0^\varepsilon,$$

and hence, using (5.28) and Proposition 3.7, we have

$$\|\mathcal{P}_{t,K+1,\delta}^\varepsilon u_0^\varepsilon - \mathcal{P}_{t,K,\delta}^\varepsilon u_0^\varepsilon\|_{L^2(\mathbb{R}^d;\mathbb{C}^N)} \leq C_{K,T} M \varepsilon^K.$$

The Theorem is proved.  $\square$

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DEPARTMENT OF MATHEMATICS, COURANT INSTITUTE OF MATHEMATICAL SCIENCES, NEW YORK UNIVERSITY, NEW YORK, NY 10012, EMAIL: JIANFENG@CIMS.NYU.EDU

DEPARTMENT OF MATHEMATICS, COURANT INSTITUTE OF MATHEMATICAL SCIENCES, NEW YORK UNIVERSITY, NEW YORK, NY 10012, EMAIL: XUYANG@CIMS.NYU.EDU