FROZEN GAUSSIAN APPROXIMATION FOR HIGH FREQUENCY WAVE PROPAGATION IN PERIODIC MEDIA

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Abstract. Propagation of high-frequency wave in periodic media is a challenging problem due to the existence of multiscale characterized by short wavelength, small lattice constant and large physical domain size. Conventional computational methods lead to extremely expensive costs, especially in high dimensions. In this paper, based on Bloch decomposition and asymptotic analysis in the phase space, we derive the frozen Gaussian approximation for high-frequency wave propagation in periodic media and establish its converge to the true solution. The formulation leads to efficient numerical algorithms, which are presented in a companion paper [5].

1. Introduction

We are interested in studying high-frequency wave propagation in periodic media. A typical example is given by the following Schrödinger equation in the semiclassical regime with a superposition of a (highly oscillatory) microscopic periodic potential and a macroscopic smooth potential,

$$\mathrm{i}\varepsilon\frac{\partial \psi^\varepsilon}{\partial t} = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + V(\boldsymbol{x}/\varepsilon)\psi^\varepsilon + U(\boldsymbol{x})\psi^\varepsilon, \qquad \boldsymbol{x}\in\mathbb{R}^d, \tag{1.1}$$

where V and U are smooth potential functions, V is periodic with respect to the lattice $\mathbb{Z}^d$: $V(\boldsymbol{x}+\mathbf{e}_i) = V(\boldsymbol{x})$ for any $\boldsymbol{x}\in\mathbb{R}^d$ and $\{\boldsymbol{e}_i,\ i=1,2,\cdots,d\}$ is the standard basis of $\mathbb{R}^d$. Here $\varepsilon \ll 1$ is the rescaled Planck constant, ψ^ε is the wave function, and d is the spatial dimensionality.

The equation (1.1) can be viewed as a model for electron dynamics in a crystal, where V is the effective periodic potential induced by the crystal, and U is some external macroscopic potential. Notice that we have identified the period of $V(\boldsymbol{x}/\varepsilon)$ and the "semiclassical parameter" in front of the derivative terms. This parameter choice gives the most interesting case as $\varepsilon\to 0$ [2].

The mathematical analysis of this work is motivated by the challenge of numerical simulation of (1.1) when ε is small. In this semiclassical regime, the wave function ψ^ε becomes oscillatory with wave length $\mathcal{O}(\varepsilon)$. This means a computational domain of order 1 size contains $\mathcal{O}(1/\varepsilon)$ wavelengths, and each of them needs to be resolved if conventional numerical methods are applied. For example, even for the simplest case $V=0$ (no lattice potential), a mesh size of $\mathcal{O}(\varepsilon)$ is required when using the time-splitting spectral method [1] to compute (1.1) directly; an even worse mesh size of $o(\varepsilon)$ is needed if one uses the Crank-Nicolson schemes [26] or the Dufort-Frankel scheme [27]. Besides, the presence of non-zero lattice potential introduces further difficulties which restrict the mesh size to be $o(\varepsilon)$ in the standard time-splitting spectral method [1]. Special techniques using Bloch decomposition are needed to relax the mesh size to be of $\mathcal{O}(\varepsilon)$ [12–14]. Moreover, in these methods, a large domain is demanded in order to

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avoid the boundary effects. Therefore the total number of grid points is huge, which usually leads to unaffordable computational cost, especially in high ($d > 1$) dimensions.

An alternative efficient approach is to solve (1.1) asymptotically by the Bloch decomposition and modified WKB methods [3, 4, 7], which lead to eikonal and transport equations in the semi-classical regime. An advantage of this method is that the computational cost is independent of ε. However, the eikonal equation can develop singularities which make the method break down at caustics. The Gaussian beam method (GBM) [31] was then introduced by Popov to overcome this drawback at caustics. The idea is to allow the phase function to be complex and choose the imaginary part properly so that the solution has a Gaussian profile; see [15–20, 28, 37, 38] for recent developments. Similar ideas can be also found in the Hagedorn wave packet method [8, 9]. Unlike the geometric optics based method, the Gaussian beam method allows for accurate computation of wave function around caustics [6, 33]. But the problem is that the constructed beam must stay near the geometric rays to maintain accuracy. This becomes a drawback when the solution spreads [23, 28, 32].

The Herman-Kluk propagator [11, 21, 22] was proposed for Schrödinger equation without the oscillatory periodic background potential. The method was rigorously analyzed in [35, 36] and further extended as the frozen Gaussian approximation (FGA) for general high frequency wave propagation in [23–25]. The FGA method uses Gaussian functions with fixed widths, instead of using those that might spread over time, to approximate the wave solution. Despite its superficial similarity with the Gaussian beam method, it is different at a fundamental level. FGA is based on phase plane analysis, while GBM is based on the asymptotic solution to a wave equation with Gaussian initial data. In FGA, the solution to the wave equation is approximated by a superposition of Gaussian functions living in phase space, and each function is not necessarily an asymptotic solution, while GBM uses Gaussian functions (called beams) in physical space, with each individual beam being an asymptotic solution to the wave equation. The main advantage of FGA over GBM is that the problem of beam spreading no longer exists.

In this paper, we extend FGA for computation of high-frequency wave propagation in periodic media. We mainly focus on the derivation of an integral representation formula of FGA in the phase space and establish the rigorous convergence results for FGA. While the FGA works for general strictly hyperbolic equations, we focus in this paper the case of semiclassical Schrödinger equation with periodic media (1.1). The computational algorithm and numerical results will be presented in a separate paper [5]. The rest of the paper is organized as follows. We first recall the Bloch decomposition of periodic media and introduce the windowed Bloch transform in Section 2. In Section 3, we present the formulation of FGA for periodic media and the main convergence result. The proof of the main result is given in Section 4.

Notations. The absolute value, Euclidean distance, vector norm, induced matrix norm, and sum of components of a multi-index will all be denoted by $|\cdot|$. We will use the standard notations $\mathcal{S}$, $\mathcal{C}^\infty$, and $\mathcal{C}_c^\infty$ for Schwartz class functions, smooth functions, and compactly supported smooth functions, respectively. We will sometimes use subscripts to specify the dependence of a constant on the parameters, for instance, notations like C_T to specify the dependence of a constant on a parameter T.

2. Bloch decomposition and windowed Bloch transform

The frozen Gaussian approximation for periodic media relies crucially on the Bloch decomposition to capture the fine scale ($\mathcal{O}(\varepsilon)$ spatial scale) oscillation. First we briefly recall the well-known Bloch-Floquet decomposition for Schrödinger operators with a periodic potential.

Consider a Schrödinger operator

$$H = -\frac{1}{2}\Delta + V(\boldsymbol{x}), \tag{2.1}$$

where the potential V is periodic with respect to the lattice $\mathbb{Z}^d$. We denote Γ the unit cell of the lattice: $\Gamma = [0,1)^d$. The unit cell of the reciprocal lattice (known as the first Brillouin zone) is given by $\Gamma^* = [-\pi, \pi)^d$. It is standard (e.g., [34]) that the spectrum of H is given by energy bands

$$\operatorname{spec}(H) = \bigcup_{n=1}^{\infty} \bigcup_{\boldsymbol{\xi}\in\Gamma^*} E_n(\boldsymbol{\xi}),$$

where for each $\boldsymbol{\xi} \in \Gamma^*$, $\{E_n(\boldsymbol{\xi})\}$ are the collection of eigenvalues (in ascending order) of the operator

$$H_{\boldsymbol{\xi}} = \frac{1}{2}(-\mathrm{i}\nabla_{\boldsymbol{x}} + \boldsymbol{\xi})^2 + V(\boldsymbol{x})$$

with periodic boundary condition on Γ. The Bloch waves are the associated eigenfunctions: For each band n and $\boldsymbol{\xi} \in \Gamma^*$, it solves

$$H_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi}, \cdot) = E_n(\boldsymbol{\xi}) u_n(\boldsymbol{\xi}, \cdot). \tag{2.2}$$

with periodic boundary condition on Γ, where $\boldsymbol{\xi}$ serves as a parameter in the above equation. $u_n(\boldsymbol{\xi}, \cdot)$ is normalized that

$$\int_\Gamma |u_n(\boldsymbol{\xi}, \boldsymbol{x})|^2 \,\mathrm{d}x = 1. \tag{2.3}$$

We extend $u_n(\boldsymbol{\xi}, \boldsymbol{x})$ periodically with respect to the second variable, so it is defined on $\Gamma^* \times \mathbb{R}^d$. We will also write $u_{n,\boldsymbol{\xi}} = u_n(\boldsymbol{\xi}, \cdot)$ when the former is more convenient.

These Bloch waves generalize the Fourier modes (complex exponentials) to periodic media (see for example discussions in [7]). In particular, for any function $f \in L^2(\mathbb{R}^d)$, we have the Bloch decomposition

$$f(\boldsymbol{x}) = \frac{1}{(2\pi)^{d/2}} \sum_{n=1}^{\infty} \int_{\Gamma^*} u_n(\boldsymbol{\xi}, \boldsymbol{x}) e^{\mathrm{i}\boldsymbol{\xi}\cdot\boldsymbol{x}} (\mathcal{B}f)_n(\boldsymbol{\xi}) \,\mathrm{d}\boldsymbol{\xi}. \tag{2.4}$$

where the Bloch transform $\mathcal{B} : L^2(\mathbb{R}^d) \to L^2(\Gamma^*)^{\mathbb{N}}$ is given by

$$(\mathcal{B}f)_n(\boldsymbol{\xi}) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \bar{u}_n(\boldsymbol{\xi}, \boldsymbol{y}) e^{-\mathrm{i}\boldsymbol{\xi}\cdot\boldsymbol{y}} f(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y}. \tag{2.5}$$

As an analog of the Parseval's identity, we have

$$\int_{\mathbb{R}^d} |f(\boldsymbol{x})|^2 \,\mathrm{d}\boldsymbol{x} = \sum_{n=1}^{\infty} \int_{\Gamma^*} |(\mathcal{B}f)_n(\boldsymbol{\xi})|^2 \,\mathrm{d}\boldsymbol{\xi}. \tag{2.6}$$

As suggested by (2.4) and (2.5), we introduce the notation Ω to denote the phase space corresponding to one band (Γ^* is viewed as a torus, *i.e.*, periodic boundary condition is assumed on Γ^*)

$$\Omega := \mathbb{R}^d \times \Gamma^* = \big\{(\boldsymbol{x}, \boldsymbol{\xi}) \mid \boldsymbol{x} \in \mathbb{R}^d,\, \boldsymbol{\xi} \in \Gamma^*\big\}. \tag{2.7}$$

Correspondingly, we will use the notation $(\boldsymbol{q}, \boldsymbol{p})$ for a point in Ω.

For later usage, we define the Berry phase $\mathcal{A}_n$ for the Bloch waves,

$$\mathcal{A}_n(\boldsymbol{\xi}) = \big\langle u_n(\boldsymbol{\xi}, \cdot), \mathrm{i}\nabla_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi}, \cdot)\big\rangle_{L^2(\Gamma)}. \tag{2.8}$$

The normalization condition (2.3) implies $\mathcal{A}_n(\boldsymbol{\xi})$ is always a real number. We should be cautious about one subtlety though as the eigenvalue equation (2.2) and the normalization only define $u_n(\boldsymbol{\xi}, \cdot)$ up to a unit complex number, in particular, for any function φ periodic in Γ^*,

$$v_n(\boldsymbol{\xi}, \boldsymbol{x}) = e^{\mathrm{i}\varphi(\boldsymbol{\xi})} u_n(\boldsymbol{\xi}, \boldsymbol{x}), \qquad (\boldsymbol{x}, \boldsymbol{\xi}) \in \Omega, \tag{2.9}$$

also provides a set of Bloch waves. This is known as the gauge choice for the Bloch waves. However, different gauge choice gives different values of $\mathcal{A}_n(\boldsymbol{\xi})$ and even causes trouble if φ is discontinuous. While for the analysis, it suffices to assume smooth dependence of u_n on $\boldsymbol{\xi}$ (which is possible as the n-th band is separated from the rest of the spectrum), this gauge freedom makes numerical computation nontrivial. We will further address this by designing a gauge-invariant algorithm in a companion paper [5] on the numerical algorithms.

Differentiating (2.2) with respect to $\boldsymbol{\xi}$ produces

$$H_{\boldsymbol{\xi}} \nabla_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi}, \boldsymbol{x}) + (-\mathrm{i}\nabla_{\boldsymbol{x}} + \boldsymbol{\xi}) u_n(\boldsymbol{\xi}, \boldsymbol{x}) = E_n(\boldsymbol{\xi}) \nabla_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi}, \boldsymbol{x}) + \nabla_{\boldsymbol{\xi}} E_n(\boldsymbol{\xi}) u_n(\boldsymbol{\xi}, \boldsymbol{x}). \tag{2.10}$$

Taking inner product with $u_n(\boldsymbol{\xi}, \cdot)$ yields

$$\nabla_{\boldsymbol{\xi}} E_n(\boldsymbol{\xi}) = -\mathrm{i}\langle u_n(\boldsymbol{\xi}, \cdot), \nabla_{\boldsymbol{x}} u_n(\boldsymbol{\xi}, \cdot)\rangle + \boldsymbol{\xi}. \tag{2.11}$$

Differentiate (2.10) with respect to $\boldsymbol{\xi}$ again gives

$$\begin{aligned} H_{\boldsymbol{\xi}} \nabla^2_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi}, \boldsymbol{x}) &+ 2(-\mathrm{i}\nabla_{\boldsymbol{x}} + \boldsymbol{\xi}) \nabla_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi}, \boldsymbol{x}) + u_n(\boldsymbol{\xi}, \boldsymbol{x}) I \\ &= E_n(\boldsymbol{\xi}) \nabla^2_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi}, \boldsymbol{x}) + 2\nabla_{\boldsymbol{\xi}} E_n(\boldsymbol{\xi}) \nabla_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi}, \boldsymbol{x}) + E_n(\boldsymbol{\xi}) \nabla^2_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi}, \boldsymbol{x}). \end{aligned} \tag{2.12}$$

Taking inner product with $u_n(\boldsymbol{\xi}, \cdot)$, one gets

$$\begin{aligned} \langle u_n(\boldsymbol{\xi}, \cdot), -\mathrm{i}\nabla_{\boldsymbol{x}} \nabla_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi}, \boldsymbol{x})\rangle &+ \boldsymbol{\xi}\langle u_n(\boldsymbol{\xi}, \cdot), \nabla_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi}, \cdot)\rangle + I/2 \\ &= \nabla_{\boldsymbol{\xi}} E_n(\boldsymbol{\xi}) \langle u_n(\boldsymbol{\xi}, \cdot), \nabla_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi}, \boldsymbol{x})\rangle + \tfrac{1}{2} E_n(\boldsymbol{\xi}) \langle u_n(\boldsymbol{\xi}, \cdot), \nabla^2_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi}, \cdot)\rangle. \end{aligned} \tag{2.13}$$

These identities (2.11) and (2.13) will be useful later.

We shall now introduce the windowed Bloch transform. This is an analog of the windowed Fourier transform (also known as the short time Fourier transform) widely used in time-frequency signal analysis.

Definition 2.1. The windowed Bloch transform $\mathcal{W} : L^2(\mathbb{R}^d) \to L^2(\Omega)^{\mathbb{N}}$ is defined as

$$(\mathcal{W} f)_n(\boldsymbol{q}, \boldsymbol{p}) = \frac{2^{d/4}}{(2\pi)^{3d/4}} \langle u_n(\boldsymbol{p}, \cdot) G_{\boldsymbol{q},\boldsymbol{p}}, f\rangle = \frac{2^{d/4}}{(2\pi)^{3d/4}} \int_{\mathbb{R}^d} \bar{u}_n(\boldsymbol{p}, \boldsymbol{x}) \bar{G}_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{x}) f(\boldsymbol{x}) \,\mathrm{d}\boldsymbol{x}, \tag{2.14}$$

where $G_{\boldsymbol{q},\boldsymbol{p}}$ is a Gaussian centered at $(\boldsymbol{q}, \boldsymbol{p}) \in \Omega$, given by

$$G_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{x}) = \exp\Bigl(-\frac{1}{2} |\boldsymbol{x} - \boldsymbol{q}|^2 + \mathrm{i}\boldsymbol{p} \cdot (\boldsymbol{x} - \boldsymbol{q})\Bigr). \tag{2.15}$$

The adjoint operator $\mathcal{W}^* : L^2(\Omega)^{\mathbb{N}} \to L^2(\mathbb{R}^d)$ is then

$$(\mathcal{W}^* g)(\boldsymbol{x}) = \frac{2^{d/4}}{(2\pi)^{3d/4}} \sum_{n=1}^{\infty} \iint_{\Omega} u_n(\boldsymbol{p}, \boldsymbol{x}) G_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{x}) g_n(\boldsymbol{q}, \boldsymbol{p}) \,\mathrm{d}\boldsymbol{q} \,\mathrm{d}\boldsymbol{p}. \tag{2.16}$$

Proposition 2.2. *The windowed Bloch transform and its adjoint satisfies*

$$\mathcal{W}^* \mathcal{W} = \mathrm{Id}_{L^2(\mathbb{R}^d)}. \tag{2.17}$$

Remark. Similar to the windowed Fourier transform, the representation given by the windowed Bloch transform is redundant, so that $\mathcal{W}\mathcal{W}^* \neq \mathrm{Id}_{L^2(\Omega)^{\mathbb{N}}}$. The normalization constant in the definition of $\mathcal{W}$ is also due to this redundancy.

Proof. Fix a $f \in L^2(\mathbb{R}^d)$, by definition, we have

$$\begin{aligned}(\mathcal{W}^*\mathcal{W}f)(\boldsymbol{x}) &= \frac{2^{d/2}}{(2\pi)^{3d/2}} \sum_{n=1}^{\infty} \iint_{\Omega} u_n(\boldsymbol{p},\boldsymbol{x}) G_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{x}) \langle G_{\boldsymbol{q},\boldsymbol{p}} u_n(\boldsymbol{p},\cdot), f\rangle \,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p} \\ &= \frac{2^{d/2}}{(2\pi)^{3d/2}} \sum_{n=1}^{\infty} \iint_{\Omega} \int_{\mathbb{R}^d} u_n(\boldsymbol{p},\boldsymbol{x}) G_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{x}) \bar{G}_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{y}) \bar{u}_n(\boldsymbol{p},\boldsymbol{y}) f(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}.\end{aligned}$$

Let us integrate in $\boldsymbol{q}$ first.

$$\begin{aligned}\int_{\mathbb{R}^d} G_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{x}) \bar{G}_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{q} &= e^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})} \int_{\mathbb{R}^d} e^{-|\boldsymbol{x}-\boldsymbol{q}|^2/2-|\boldsymbol{y}-\boldsymbol{q}|^2/2} \,\mathrm{d}\boldsymbol{q} \\ &= e^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})} e^{-|\boldsymbol{x}-\boldsymbol{y}|^2/4} \int_{\mathbb{R}^d} \exp\left(-\left|\boldsymbol{q} - \frac{\boldsymbol{x}+\boldsymbol{y}}{2}\right|^2\right) \mathrm{d}\boldsymbol{q} \\ &= \pi^{d/2} e^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})} e^{-|\boldsymbol{x}-\boldsymbol{y}|^2/4}.\end{aligned}$$

Hence, denoting $\widetilde{f}_{\boldsymbol{x}}(\boldsymbol{y}) = e^{-|\boldsymbol{x}-\boldsymbol{y}|^2/4} f(\boldsymbol{y})$, we have

$$\begin{aligned}(\mathcal{W}^*\mathcal{W}f)(\boldsymbol{x}) &= \frac{1}{(2\pi)^d} \sum_{n=1}^{\infty} \int_{\Gamma^*} \int_{\mathbb{R}^d} u_n(\boldsymbol{p},\boldsymbol{x}) e^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})} e^{-|\boldsymbol{x}-\boldsymbol{y}|^2/4} \bar{u}_n(\boldsymbol{p},\boldsymbol{y}) f(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{p} \\ &= \frac{1}{(2\pi)^d} \sum_{n=1}^{\infty} \int_{\Gamma^*} \int_{\mathbb{R}^d} u_n(\boldsymbol{p},\boldsymbol{x}) e^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})} \bar{u}_n(\boldsymbol{p},\boldsymbol{y}) \widetilde{f}_{\boldsymbol{x}}(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{p} \\ &\overset{(2.4)}{=} \widetilde{f}_{\boldsymbol{x}}(\boldsymbol{x}) = e^{-|\boldsymbol{x}-\boldsymbol{x}|^2/4} f(\boldsymbol{x}) = f(\boldsymbol{x}).\end{aligned}$$

□

The previous proposition motivates us to consider the contribution of each band to the reconstruction formulae (2.17). This gives to the operator $\Pi_n^{\mathcal{W}} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ for each $n \in \mathbb{N}$

$$(\Pi_n^{\mathcal{W}} f)(\boldsymbol{x}) = \frac{2^{d/4}}{(2\pi)^{3d/4}} \iint_{\Omega} u_n(\boldsymbol{p},\boldsymbol{x}) G_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{x}) (\mathcal{W}f)_n(\boldsymbol{q},\boldsymbol{p}) \,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}. \tag{2.18}$$

It follows from (2.17) that $\sum_n \Pi_n^{\mathcal{W}} = \mathrm{Id}_{L^2(\mathbb{R}^d)}$, while $\Pi_n^{\mathcal{W}}$ is not projection due to the redundancy of windowed Bloch transform.

3. Formulation and main results

Let us start with fixing some more notations. We will switch between physical domain and phase space in the FGA formulation. For clarity, we will use $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$ as spatial variables, $(\boldsymbol{q}, \boldsymbol{p}) \in \mathbb{R}^{2d}$ as phase space variables. The capital letters $\boldsymbol{X}$ and $\boldsymbol{Y}$ are shorthand notations for $\boldsymbol{X} = \boldsymbol{x}/\varepsilon$ and $\boldsymbol{Y} = \boldsymbol{y}/\varepsilon$.

We define an effective (classical) Hamiltonian corresponding to each energy band by

$$h_n(\boldsymbol{q},\boldsymbol{p}) = E_n(\boldsymbol{p}) + U(\boldsymbol{q}). \tag{3.1}$$

The associated Hamiltonian flow $\kappa_n(t) = (\boldsymbol{Q}_n(t,\boldsymbol{q},\boldsymbol{p}), \boldsymbol{P}_n(t,\boldsymbol{q},\boldsymbol{p}))$ solves

$$\begin{cases} \dfrac{d\boldsymbol{Q}_n}{dt} = \nabla_{\boldsymbol{P}_n} h_n(\boldsymbol{Q}_{\boldsymbol{n}}, \boldsymbol{P}_n), \\ \dfrac{d\boldsymbol{P}_n}{dt} = -\nabla_{\boldsymbol{Q}_n} \boldsymbol{Q}_n, \boldsymbol{P}_n) \end{cases} \tag{3.2}$$

on Ω with initial conditions $\boldsymbol{Q}_n(0,\boldsymbol{q},\boldsymbol{p}) = \boldsymbol{q}$ and $\boldsymbol{P}_n(0,\boldsymbol{q},\boldsymbol{p}) = \boldsymbol{p}$.

From now on, we will use the short hand notation $(\boldsymbol{Q}_n, \boldsymbol{P}_n)$ for $(\boldsymbol{Q}_n(t,\boldsymbol{q},\boldsymbol{p}), \boldsymbol{P}_n(t,\boldsymbol{q},\boldsymbol{p}))$. For the long time existence of the Hamiltonian flow (3.2), we will assume that the external potential $U(\boldsymbol{x})$ is subquadratic as below.

Definition 3.1. A potential U is called *subquadratic*, if $\|\partial_{\boldsymbol{x}}^{\alpha} U(\boldsymbol{x})\|_{L^\infty}$ is finite for all multi-index $|\alpha| \geq 2$.

Remark. As a result, since the domain Γ^* for $\boldsymbol{p}$ is bounded, the Hamiltonian h_n is also subquadratic.

The frozen Gaussian approximation will be formulated by the following Fourier integral operator.

Definition 3.2. (Fourier Integral Operator) For $u \in \mathcal{S}(\mathbb{R}^{2d} \times \Omega, \mathbb{C})$ and $\varphi \in \mathcal{S}(\mathbb{R}^d, \mathbb{C})$ we define the Fourier Integral Operator with symbol u by the oscillatory integral

$$[\mathcal{I}^\varepsilon(u)\varphi](\boldsymbol{x}) = \frac{1}{(2\pi\varepsilon)^{3d/2}} \iint_{\Omega} \int_{\mathbb{R}^d} e^{\frac{\mathrm{i}}{\varepsilon}\Phi(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})} u(\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})\varphi(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y} \,\mathrm{d}\boldsymbol{q} \,\mathrm{d}\boldsymbol{p} \tag{3.3}$$

where the complex valued phase function $\Phi(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})$ is given by

$$\Phi(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p}) = S(t,\boldsymbol{q},\boldsymbol{p}) - \boldsymbol{p}\cdot(\boldsymbol{y}-\boldsymbol{q}) + \boldsymbol{P}\cdot(\boldsymbol{x}-\boldsymbol{Q}) + \frac{\mathrm{i}}{2}|\boldsymbol{y}-\boldsymbol{q}|^2 + \frac{\mathrm{i}}{2}|\boldsymbol{x}-\boldsymbol{Q}|^2 \tag{3.4}$$

and $S(t,\boldsymbol{q},\boldsymbol{p})$ is a real-valued *action* function associated to κ satisfying

$$\nabla_{\boldsymbol{q}} S(t,\boldsymbol{q},\boldsymbol{p}) = -\boldsymbol{p} + \nabla_{\boldsymbol{q}}\boldsymbol{Q}\cdot\boldsymbol{P}, \qquad \nabla_{\boldsymbol{p}} S(t,\boldsymbol{q},\boldsymbol{p}) = \nabla_{\boldsymbol{p}}\boldsymbol{Q}\cdot\boldsymbol{P}. \tag{3.5}$$

Note that if $\kappa(t) = \kappa_n(t)$, the action $S_n(t,\boldsymbol{q},\boldsymbol{p})$ can be obtained by solving the evolution equation

$$\frac{dS_n}{dt} = \boldsymbol{P}_n \cdot \nabla_{\boldsymbol{P}_n} h_n(\boldsymbol{Q}_n,\boldsymbol{P}_n) - h_n(\boldsymbol{Q}_n,\boldsymbol{P}_n), \tag{3.6}$$

with initial condition $S_n(0,\boldsymbol{q},\boldsymbol{p}) = 0$.

We are now ready to formulate the frozen Gaussian approximation. The FGA approximates the solution of the Schrödinger equation (1.1) on the n-th band to the leading order by

$$\psi^\varepsilon_{\mathrm{FGA}}(t,\boldsymbol{x}) = \left[\mathcal{I}^\varepsilon\left(a_{n,0}(t,\boldsymbol{q},\boldsymbol{p})u_n(\boldsymbol{P}_n,\frac{\boldsymbol{x}}{\varepsilon})\bar{u}_n(\boldsymbol{p},\frac{\boldsymbol{y}}{\varepsilon})\right)\psi_0^\varepsilon\right](\boldsymbol{x}), \tag{3.7}$$

where ψ_0^ε is the initial condition. More explicitly, at time t, $\psi^\varepsilon_{\mathrm{FGA}}$ is given by

$$\begin{aligned}\psi^\varepsilon_{\mathrm{FGA}}(t,\boldsymbol{x}) = \frac{1}{(2\pi\varepsilon)^{3d/2}} \iint_{\Omega} a_{n,0}(t,\boldsymbol{q},\boldsymbol{p}) e^{\mathrm{i}S_n(t,\boldsymbol{q},\boldsymbol{p})/\varepsilon} G^\varepsilon_{\boldsymbol{Q}_n,\boldsymbol{P}_n}(\boldsymbol{x}) u_n(\boldsymbol{P}_n,\boldsymbol{x}/\varepsilon) \\ \cdot \langle G^\varepsilon_{\boldsymbol{q},\boldsymbol{p}} u_n(\boldsymbol{p},\cdot/\varepsilon), \psi_0^\varepsilon\rangle \,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}.\end{aligned} \tag{3.8}$$

Here and in the sequel, we use the short-hand notation for Gaussians with semiclassical scaling

$$G^\varepsilon_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{x}) := \exp\left(-\frac{|\boldsymbol{x}-\boldsymbol{q}|^2}{2\varepsilon} + \mathrm{i}\frac{\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{q})}{\varepsilon}\right), \tag{3.9}$$

where the subscripts $(\boldsymbol{q},\boldsymbol{p})$ indicate the center of the Gaussian in phase space. Note that the semiclassical Fourier transform of $G^\varepsilon_{\boldsymbol{q},\boldsymbol{p}}$ is

$$\widehat{G}^\varepsilon_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{\xi}) = \frac{1}{(2\pi\varepsilon)^{d/2}} \int_{\mathbb{R}^d} G^\varepsilon_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{x}) e^{-\mathrm{i}\boldsymbol{\xi}\cdot\boldsymbol{x}/\varepsilon}\,\mathrm{d}\boldsymbol{x} = \exp\left(-\frac{|\boldsymbol{\xi}-\boldsymbol{p}|^2}{2\varepsilon} + \mathrm{i}\frac{\boldsymbol{q}\cdot(\boldsymbol{\xi}-\boldsymbol{p})}{\varepsilon}\right). \tag{3.10}$$

Correspondingly, the semiclassical windowed Bloch transform $\mathcal{W}^\varepsilon : L^2(\mathbb{R}^d) \to L^2(\Omega)^{\mathbb{N}}$ is defined as

$$(\mathcal{W}^\varepsilon f)_n(\boldsymbol{q},\boldsymbol{p}) = \frac{2^{d/4}}{(2\pi\varepsilon)^{3d/4}} \left\langle u_n(\boldsymbol{p},\cdot/\varepsilon)G^\varepsilon_{\boldsymbol{q},\boldsymbol{p}}, f\right\rangle = \frac{2^{d/4}}{(2\pi\varepsilon)^{3d/4}} \int_{\mathbb{R}^d} \bar{u}_n(\boldsymbol{p},\boldsymbol{x}/\varepsilon)\bar{G}^\varepsilon_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{x}) f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}. \tag{3.11}$$

Similarly we also have the operator $\Pi_n^{\mathcal{W},\varepsilon} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ for each $n \in \mathbb{N}$ with semiclassical scaling

$$(\Pi_n^{\mathcal{W},\varepsilon} f)(\boldsymbol{y}) = \frac{2^{d/4}}{(2\pi\varepsilon)^{3d/4}} \iint_{\Omega} u_n(\boldsymbol{\xi},\boldsymbol{y}/\varepsilon) G^\varepsilon_{\boldsymbol{x},\boldsymbol{\xi}}(\boldsymbol{y}) (\mathcal{W}^\varepsilon f)_n(\boldsymbol{x},\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{\xi}. \tag{3.12}$$

It follows from (2.17) and a change of variable that $\sum_n \Pi_n^{\mathcal{W},\varepsilon} = \mathrm{Id}_{L^2(\mathbb{R}^d)}$.

The only term in (3.8) that remains to be specified is the amplitude $a_{n,0}(t,\boldsymbol{q},\boldsymbol{p})$. It solves the evolution equation

$$\begin{aligned}\partial_t a_{n,0} = -\mathrm{i} a_{n,0}\mathcal{A}_n(\boldsymbol{P}_n)\cdot\nabla U(\boldsymbol{Q}_n) + \frac{1}{2} a_{n,0}\,\mathrm{tr}\left(\partial_{\boldsymbol{z}}\boldsymbol{P}_n\,\nabla^2 E(\boldsymbol{P}_n)\big(Z_n\big)^{-1}\right)\\ - \frac{\mathrm{i}}{2} a_{n,0}\,\mathrm{tr}\left(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n\,\nabla^2 U(\boldsymbol{Q}_n)\big(Z_n\big)^{-1}\right),\end{aligned} \tag{3.13}$$

with initial conditions $a_{n,0}(0,\boldsymbol{q},\boldsymbol{p}) = 2^{d/2}$ for each $(\boldsymbol{q},\boldsymbol{p})$ and we recall that $\mathcal{A}_n(\boldsymbol{\xi}) = \langle u_n(\boldsymbol{\xi},\cdot), \mathrm{i}\nabla_{\boldsymbol{\xi}} u_n(\boldsymbol{\xi},\cdot)\rangle$ is the Berry phase. Here the matrix Z associated with the Hamiltonian flow $\kappa_n(t)$ is defined by

$$Z_n(t,q,p) := \partial_{\boldsymbol{z}}\left(\boldsymbol{Q}_n + \mathrm{i}\boldsymbol{P}_n\right), \tag{3.14}$$

where $\partial_{\boldsymbol{z}} := \partial_{\boldsymbol{q}} - \mathrm{i}\partial_{\boldsymbol{p}}$.

We now state the main results of this work.

Theorem 3.1. *Assume that the n-th Bloch band $E_n(\boldsymbol{\xi})$ does not intersect any other Bloch bands for all $\boldsymbol{\xi}\in\Gamma^*$ and the Hamiltonian $h_n(\boldsymbol{x},\boldsymbol{\xi})$ is subquadratic. Let $\mathscr{U}_t^\varepsilon$ be the propagator of the time-dependent Schrödinger equation* (1.1) *with initial condition $\psi_0^\varepsilon \in L^2(\mathbb{R}^d)$. Then for any given T, $0\le t\le T$ and sufficiently small ε, we have*

$$\sup_{0\le t\le T}\left\| \mathscr{U}_t^\varepsilon\big(\Pi_n^{\mathcal{W},\varepsilon}\psi_0^\varepsilon\big) - \mathcal{I}^\varepsilon\big(a_{n,0}u_n(\boldsymbol{P}_n,\boldsymbol{x}/\varepsilon)\bar{u}_n(\boldsymbol{p},\boldsymbol{y}/\varepsilon)\big)\psi_0^\varepsilon\right\|_{L^2} \le C_{T,n}\,\varepsilon\,\big\|\psi_0^\varepsilon\big\|_{L^2}. \tag{3.15}$$

Remark. Note that the FGA solution approximates the time evolution of $\Pi_n^{\mathcal{W},\varepsilon}\psi_0^\varepsilon$, which is the n-th band contribution to the initial condition in the reconstruction formulae (2.17). In particular, if the initial condition is concentrated on the n-th band in the sense that $\psi_0^\varepsilon = \Pi_n^{\mathcal{W},\varepsilon}\psi_0^\varepsilon$, the theorem states that the solution to (1.1) is approximated by the FGA solution with $\mathcal{O}(\varepsilon)$ error.

Remark. We can also construct higher order approximations by replacing the term $a_{n,0}u_n(\boldsymbol{P}_n,\boldsymbol{x}/\varepsilon)$ with an ε-expansion of the form $b_{n,0}+\varepsilon b_{n,1}+\varepsilon^2 b_{n,2}+\ldots+\varepsilon^{N-1}b_{n,N-1}$ where $b_{n,0} = a_{n,0}u_n(\boldsymbol{P}_n,\boldsymbol{x}/\varepsilon)$. This will give an approximate solution $\psi_{\mathrm{FGA}}^{\varepsilon,N}$ to $\mathcal{O}(\varepsilon^N)$ accuracy. In this paper we shall focus on the first order approximation and omit the formulation and proof for higher orders.

Remark. Let us also remark that while we take the more explicit approach of using Bloch waves in a modified FGA ansatz for periodic media, as in (3.8). The same approximation can be also derived by first projecting the whole Schrödinger equation using a super-adiabatic projection as developed in [29,30] and then apply the frozen Gaussian approximation to the resulting dynamics. We will not go into the details in this work.

The proof of Theorem 3.1 is given in Section 4. By linearity of (1.1), we have the following more general statement, as an easy corollary from Theorem 3.1.

Theorem 3.2. *Assume that the first N Bloch bands $E_n(\boldsymbol{\xi})$, $n=1,\cdots,N$ do not intersect and are separated from the other bands for all $\boldsymbol{\xi}\in\Gamma^*$; and assume that the Hamiltonian $h_n(\boldsymbol{x},\boldsymbol{\xi})$ is subquadratic. Let $\mathscr{U}_t^\varepsilon$ be the propagator of the time-dependent Schrödinger equation* (1.1) *with initial condition $\psi_0^\varepsilon \in L^2(\mathbb{R}^d)$. Then for any given T, $0\le t\le T$ and sufficiently small ε, we have*

$$\begin{aligned}\sup_{0\le t\le T}\left\| \mathscr{U}_t^\varepsilon\psi_0^\varepsilon - \sum_{n=1}^{N}\mathcal{I}^\varepsilon\big(a_{n,0}u_n(\boldsymbol{P}_n,\boldsymbol{x}/\varepsilon)\bar{u}_n(\boldsymbol{p},\boldsymbol{y}/\varepsilon)\big)\psi_0^\varepsilon\right\|_{L^2}\\ \le C_{T,N}\,\varepsilon\big\|\psi_0^\varepsilon\big\|_{L^2} + \left\|\psi_0^\varepsilon - \sum_{n=1}^{N}\Pi_n^{\mathcal{W},\varepsilon}\psi_0^\varepsilon\right\|_{L^2}.\end{aligned} \tag{3.16}$$

Proof. Taking the short-hand notation $\psi^\varepsilon_{0,n} = \Pi_n^{\mathcal{W},\varepsilon}\psi_0^\varepsilon$ and $\mathscr{V}^\varepsilon_{t,n} = \mathcal{I}^\varepsilon\big(a_{n,0}u_n(\boldsymbol{P}_n, \boldsymbol{x}/\varepsilon)\bar{u}_n(\boldsymbol{p},\boldsymbol{y}/\varepsilon)\big)$, we have

$$\begin{aligned}
\left\|\mathscr{U}_t^\varepsilon\psi_0^\varepsilon - \sum_{n=1}^N \mathscr{V}^\varepsilon_{t,n}\psi_0^\varepsilon\right\|_{L^2} &= \left\|\mathscr{U}_t^\varepsilon\left(\sum_{n=1}^\infty \psi^\varepsilon_{0,n}\right) - \sum_{n=1}^N \mathscr{V}^\varepsilon_{t,n}\psi_0^\varepsilon\right\|_{L^2} \\
&= \left\|\mathscr{U}_t^\varepsilon\left(\sum_{n=1}^N \psi^\varepsilon_{0,n}\right) + \mathscr{U}_t^\varepsilon\left(\sum_{n=N+1}^\infty \psi^\varepsilon_{0,n}\right) - \sum_{n=1}^N \mathscr{V}^\varepsilon_{t,n}\psi_0^\varepsilon\right\|_{L^2} \\
&\le \left\|\mathscr{U}_t^\varepsilon\left(\sum_{n=1}^N \psi^\varepsilon_{0,n}\right) - \sum_{n=1}^N \mathscr{V}^\varepsilon_{t,n}\psi_0^\varepsilon\right\|_{L^2} + \left\|\mathscr{U}_t^\varepsilon\left(\sum_{n=N+1}^\infty \psi^\varepsilon_{0,n}\right)\right\|_{L^2} \\
&\overset{(3.15)}{\le} \sum_{n=1}^N C_{T,n}\varepsilon\left\|\psi^\varepsilon_{n,0}\right\|_{L^2} + \left\|\sum_{n=N+1}^\infty \psi_0^\varepsilon\right\|_{L^2} \\
&\le C_{T,N}\varepsilon\left\|\psi_0^\varepsilon\right\|_{L^2} + \left\|\psi_0^\varepsilon - \sum_{n=1}^N \Pi_n^{\mathcal{W},\varepsilon}\psi_0^\varepsilon\right\|_{L^2}.
\end{aligned}$$

□

4. Analysis of frozen Gaussian approximation in periodic media

4.1. **Initial condition.** Let us first study the initial condition for the frozen Gaussian approximation. At time $t = 0$, observe that by setting $t = 0$ in (3.8) we have

$$\psi^\varepsilon_{FGA,n}(0,\boldsymbol{x}) = \frac{2^{d/2}}{(2\pi\varepsilon)^{3d/2}}\iint_\Omega u_n(\boldsymbol{p},\boldsymbol{x}/\varepsilon)G^\varepsilon_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{x})\langle G^\varepsilon_{\boldsymbol{q},\boldsymbol{p}}u_n(\boldsymbol{p},\cdot/\varepsilon),\psi_0^\varepsilon\rangle\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p} = \Pi_n^{\mathcal{W},\varepsilon}\psi_0^\varepsilon$$

by definition of the operator $\Pi_n^{\mathcal{W},\varepsilon}$. Hence, the FGA solution matches $\Pi_n^{\mathcal{W},\varepsilon}\psi_0^\varepsilon$ at $t = 0$.

4.2. **Estimates of the Hamiltonian flows.** To control the error for $t > 0$, we collect here some preliminary results on the estimate of quantities associated with the Hamiltonian flows. We will assume throughout the rest of the paper that the assumptions of Theorem 3.1 hold for a fixed Bloch band n.

The following notation is useful in the proof. For $u \in \mathcal{C}^\infty(\Omega,\mathbb{C})$, we define for $k \in \mathbb{N}$,

$$M_k[u] = \max_{|\alpha_q|+|\alpha_p|\le k}\ \sup_{(\boldsymbol{q},\boldsymbol{p})\in\Omega}\left|\partial_{\boldsymbol{q}}^{\alpha_q}\partial_{\boldsymbol{p}}^{\alpha_p}u(\boldsymbol{q},\boldsymbol{p})\right| \tag{4.1}$$

where α_q and α_p are multi-indices corresponding to $\boldsymbol{q}$ and $\boldsymbol{p}$, respectively.

Definition 4.1. (Canonical Transformation) Let $\kappa : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ be a differentiable map $\kappa(\boldsymbol{q},\boldsymbol{p}) = (\boldsymbol{Q}(\boldsymbol{q},\boldsymbol{p}),\boldsymbol{P}(\boldsymbol{q},\boldsymbol{p}))$ and denote the Jacobian matrix as

$$(F) = \begin{pmatrix} (\partial_{\boldsymbol{q}}\boldsymbol{Q})^T(\boldsymbol{q},\boldsymbol{p}) & (\partial_{\boldsymbol{p}}\boldsymbol{Q})^T(\boldsymbol{q},\boldsymbol{p}) \\ (\partial_{\boldsymbol{q}}\boldsymbol{P})^T(\boldsymbol{q},\boldsymbol{p}) & (\partial_{\boldsymbol{p}}\boldsymbol{P})^T(\boldsymbol{q},\boldsymbol{p}) \end{pmatrix}. \tag{4.2}$$

We say κ is a *canonical transformation* if F is symplectic for any $(\boldsymbol{q},\boldsymbol{p}) \in \mathbb{R}^{2d}$, i.e.

$$(F)^T\begin{pmatrix} 0 & \mathrm{Id}_d \\ -\mathrm{Id}_d & 0 \end{pmatrix}F = \begin{pmatrix} 0 & \mathrm{Id}_d \\ -\mathrm{Id}_d & 0 \end{pmatrix}. \tag{4.3}$$

It is easy to check by the definition that the map $\kappa_n(t) : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ defined by $(\boldsymbol{q},\boldsymbol{p}) \to (\boldsymbol{Q}_n(t,\boldsymbol{q},\boldsymbol{p}),\boldsymbol{P}_n(t,\boldsymbol{q},\boldsymbol{p}))$ solving (3.2) is a canonical transformation.

Proposition 4.2. *We have for all $k \geq 0$*

$$\sup_{t\in[0,T]} M_k\left[F_n(t)\right] < \infty \qquad \sup_{t\in[0,T]} M_k\left[\frac{\mathrm{d}}{\mathrm{d}t}F_n(t)\right] < \infty. \tag{4.4}$$

Proof. Differentiating $F_n(t,\boldsymbol{q},\boldsymbol{p})$ with respect to t gives

$$\frac{\mathrm{d}}{\mathrm{d}t}F_n(t,\boldsymbol{q},\boldsymbol{p}) = \begin{pmatrix} \partial_{\boldsymbol{P}}\partial_{\boldsymbol{Q}}h_n & \partial_{\boldsymbol{P}}\partial_{\boldsymbol{P}}h_n \\ -\partial_{\boldsymbol{Q}}\partial_{\boldsymbol{Q}}h_n & -\partial_{\boldsymbol{Q}}\partial_{\boldsymbol{P}}h_n \end{pmatrix} F_n(t,\boldsymbol{q},\boldsymbol{p}). \tag{4.5}$$

By our assumption that U is subquadratic on $\mathbb{R}^d$ and since $E_n \in \mathcal{C}^\infty(\Gamma^*)$, there exists a constant C independent of $(\boldsymbol{q},\boldsymbol{p})$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}|F_n(t,\boldsymbol{q},\boldsymbol{p})| = \left|\begin{pmatrix} \partial_{\boldsymbol{P}}\partial_{\boldsymbol{Q}}h_n & \partial_{\boldsymbol{P}}\partial_{\boldsymbol{P}}h_n \\ -\partial_{\boldsymbol{Q}}\partial_{\boldsymbol{Q}}h_n & -\partial_{\boldsymbol{Q}}\partial_{\boldsymbol{P}}h_n \end{pmatrix}\right| \big|F_n(t,\boldsymbol{q},\boldsymbol{p})\big| \leq C\big|F_n(t,\boldsymbol{q},\boldsymbol{p})\big| \tag{4.6}$$

with $|F_n(0)| = |\mathrm{Id}_{2d}|$. By an application of Gronwall's inequality, we obtain

$$|F_n(t)| \leq e^{C|t|}. \tag{4.7}$$

Differentiating (4.5) with respect to $(\boldsymbol{q},\boldsymbol{p})$ yields

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\partial_{\boldsymbol{q}}^{\alpha_{\boldsymbol{q}}}\partial_{\boldsymbol{p}}^{\alpha_{\boldsymbol{p}}}F_n(t,\boldsymbol{q},\boldsymbol{p}) = \sum_{\beta_{\boldsymbol{q}}\leq\alpha_{\boldsymbol{q}},\beta_{\boldsymbol{p}}\leq\alpha_{\boldsymbol{p}}} \binom{\alpha_{\boldsymbol{q}}}{\beta_{\boldsymbol{q}}}\binom{\alpha_{\boldsymbol{p}}}{\beta_{\boldsymbol{p}}}\partial_{\boldsymbol{q}}^{\beta_{\boldsymbol{q}}}\partial_{\boldsymbol{p}}^{\beta_{\boldsymbol{p}}}\begin{pmatrix} \partial_{\boldsymbol{P}}\partial_{\boldsymbol{Q}}h_n & \partial_{\boldsymbol{P}}\partial_{\boldsymbol{P}}h_n \\ -\partial_{\boldsymbol{Q}}\partial_{\boldsymbol{Q}}h_n & -\partial_{\boldsymbol{Q}}\partial_{\boldsymbol{P}}h_n \end{pmatrix} \times \\ \times\, \partial_{\boldsymbol{q}}^{\alpha_{\boldsymbol{q}}-\beta_{\boldsymbol{q}}}\partial_{\boldsymbol{p}}^{\alpha_{\boldsymbol{p}}-\beta_{\boldsymbol{p}}}F_n(t,\boldsymbol{q},\boldsymbol{p}).\end{aligned} \tag{4.8}$$

Our estimate now follows by induction. □

Recall that the matrix $Z_n(t,\boldsymbol{q},\boldsymbol{p})$ is defined by

$$Z_n(t,\boldsymbol{q},\boldsymbol{p}) := \partial_{\boldsymbol{z}}\left(\boldsymbol{Q}_n(t,\boldsymbol{q},\boldsymbol{p}) + \mathrm{i}\boldsymbol{P}_n(t,\boldsymbol{q},\boldsymbol{p})\right) = \left(\partial_{\boldsymbol{q}} - \mathrm{i}\partial_{\boldsymbol{p}}\right)\left(\boldsymbol{Q}_n(t,\boldsymbol{q},\boldsymbol{p}) + \mathrm{i}\boldsymbol{P}_n(t,\boldsymbol{q},\boldsymbol{p})\right). \tag{4.9}$$

We have the following. It follows the same proof of [23, Proposition 3.5], which we reproduce here for completeness.

Proposition 4.3. *$Z_n(t,\boldsymbol{q},\boldsymbol{p})$ is invertible for $(\boldsymbol{q},\boldsymbol{p}) \in \Omega$. Moreover, for each $k \in \mathbb{N}$,*

$$M_k\Big[\big(Z_n(t)\big)^{-1}\Big] < \infty. \tag{4.10}$$

Proof. $Z_n(t,\boldsymbol{q},\boldsymbol{p})$ inherits the property that $M_k(Z_n(t,\boldsymbol{q},\boldsymbol{p})) < \infty$ from the same estimate for $F_n(t,\boldsymbol{q},\boldsymbol{p})$. Moreover, we have

$$\begin{aligned} Z_n(Z_n)^*(t,\boldsymbol{q},\boldsymbol{p}) &= \begin{pmatrix}\mathrm{i}\,\mathrm{Id}_d & \mathrm{Id}_d\end{pmatrix}(F_n)^T(t,\boldsymbol{q},\boldsymbol{p})\begin{pmatrix}\mathrm{Id}_d & -\mathrm{i}\,\mathrm{Id}_d \\ \mathrm{i}\,\mathrm{Id}_d & \mathrm{Id}_d\end{pmatrix}F_n(t,\boldsymbol{q},\boldsymbol{p})\begin{pmatrix}-\mathrm{i}\,\mathrm{Id}_d \\ \mathrm{Id}_d\end{pmatrix} \\ &= \begin{pmatrix}\mathrm{i}\,\mathrm{Id}_d & \mathrm{Id}_d\end{pmatrix}\left((F_n)^T(F_n)\right)(t,\boldsymbol{q},\boldsymbol{p})\begin{pmatrix}-\mathrm{i}\,\mathrm{Id}_d \\ \mathrm{Id}_d\end{pmatrix} \\ &\quad + \begin{pmatrix}\mathrm{i}\,\mathrm{Id}_d & \mathrm{Id}_d\end{pmatrix}(F_n)^T(t,\boldsymbol{q},\boldsymbol{p})\begin{pmatrix}0 & -\mathrm{i}\,\mathrm{Id}_d \\ \mathrm{i}\,\mathrm{Id}_d & 0\end{pmatrix}F_n(t,\boldsymbol{q},\boldsymbol{p})\begin{pmatrix}-\mathrm{i}\,\mathrm{Id}_d \\ \mathrm{Id}_d\end{pmatrix} \\ &= \begin{pmatrix}\mathrm{i}\,\mathrm{Id}_d & \mathrm{Id}_d\end{pmatrix}\left((F_n)^TF_n\right)(t,\boldsymbol{q},\boldsymbol{p})\begin{pmatrix}-\mathrm{i}\,\mathrm{Id}_d \\ \mathrm{Id}_d\end{pmatrix} + 2\,\mathrm{Id}_d\,. \end{aligned} \tag{4.11}$$

This calculation shows that, since $(F_n(t))^TF_n(t)$ is semi-positive definite, for any $\boldsymbol{v} \in \mathbb{C}^{2d}$,

$$\boldsymbol{v}^*Z_n(t)(Z_n(t))^*\boldsymbol{v} \geq 2|\boldsymbol{v}|^2. \tag{4.12}$$

Therefore $Z_n(t,\boldsymbol{q},\boldsymbol{p})$ is invertible and $\det\big(Z_n(t)\big)$ is uniformly bounded away from 0 for all $\boldsymbol{q}$ and $\boldsymbol{p}$, so by representing $(Z_n)^{-1}(t,\boldsymbol{q},\boldsymbol{p})$ by minors, $M_k\big((Z_n)^{-1}(t,\boldsymbol{q},\boldsymbol{p})\big) < \infty$, as $M_k(Z_n(t,\boldsymbol{q},\boldsymbol{p}))$ is. □

Proposition 4.4. *For each* $k \in \mathbb{N}$,

$$\sup_{t\in[0,T]} M_k\left[u_n(\boldsymbol{P}_n,\boldsymbol{x})\right] < \infty. \tag{4.13}$$

Proof. $u_n(\boldsymbol{P}_n,\boldsymbol{x})$ is smooth on the compact set $\Gamma^*\times\Gamma$ since the n-th band is separated from the rest of the spectrum (see e.g., [34, Sec XIII.16]). Thus $u_n(\boldsymbol{P}_n,\boldsymbol{x})$ is uniformly bounded on $\Gamma^*\times\Gamma$ and hence $\Gamma^*\times\mathbb{R}^d$ due to periodicity. We also see from Proposition 4.2 that the derivatives of $u_n(\boldsymbol{P}_n,\boldsymbol{x})$ are also bounded. Thus, $M_k[u_n(\boldsymbol{P}_n,\boldsymbol{x})] < \infty$ for any finite time t. □

4.3. **Higher order asymptotic solution.** To prove the theorem, we will need to construct a solution to the Schrödinger equation that is accurate up to $\mathcal{O}(\varepsilon^2)$. The construction is based on matched asymptotic expansion. Let us fix a band $n\in\mathbb{N}$ and consider the ansatz

$$\psi^\varepsilon_{\mathrm{FGA},\infty} = \frac{1}{(2\pi\varepsilon)^{3d/2}}\iint_\Omega b^\varepsilon(t,\boldsymbol{X},\boldsymbol{q},\boldsymbol{p}) G^\varepsilon_{\boldsymbol{Q}_n,\boldsymbol{P}_n} e^{\mathrm{i}S_n/\varepsilon}\left\langle G^\varepsilon_{\boldsymbol{q},\boldsymbol{p}} u_n(\boldsymbol{p},\cdot/\varepsilon),\psi_0\right\rangle \mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}, \tag{4.14}$$

where the coefficient b assumes the asymptotic expansion

$$\begin{aligned} b^\varepsilon(t,\boldsymbol{X},\boldsymbol{q},\boldsymbol{p}) &:= \sum_{j=0}^\infty \varepsilon^j b_j(t,\boldsymbol{X},\boldsymbol{q},\boldsymbol{p}) \\ &= a_{n,0}(t,\boldsymbol{q},\boldsymbol{p})u_n(\boldsymbol{P}_n,\boldsymbol{X}) \\ &\quad + \varepsilon\big(a_{n,1}(t,\boldsymbol{q},\boldsymbol{p})u_n(\boldsymbol{P}_n,\boldsymbol{X}) + b^\perp_{n,1}(t,\boldsymbol{X},\boldsymbol{q},\boldsymbol{p})\big) \\ &\quad + \varepsilon^2\big(a_{n,2}(t,\boldsymbol{q},\boldsymbol{p})u_n(\boldsymbol{P}_n,\boldsymbol{X}) + b^\perp_{n,2}(t,\boldsymbol{X},\boldsymbol{q},\boldsymbol{p})\big) + \sum_{j=3}^\infty \varepsilon^j b_j(t,\boldsymbol{X},\boldsymbol{q},\boldsymbol{p}) \end{aligned} \tag{4.15}$$

To determine the terms in the expansion, we will make use of the following Lemma.

Definition 4.5. For $f = f(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})$ and $g = g(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})$ such that for any t and $\boldsymbol{x}$,

$$f(t,\boldsymbol{x},\cdot,\cdot,\cdot), g(t,\boldsymbol{x},\cdot,\cdot,\cdot) \in L^\infty(\mathbb{R}^d;\mathcal{S}(\mathbb{R}^d\times\Gamma^*)),$$

we say that f and g are equivalent for the n-th Bloch band, denoted as $f\sim_n g$ if for any $t\geq 0$ and $\Psi_0\in L^2(\mathbb{R}^d)$

$$\iint_\Omega\int_{\mathbb{R}^d}(f-g)(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})G^\varepsilon_{\boldsymbol{Q}_n,\boldsymbol{P}_n}e^{\mathrm{i}S_n(t,\boldsymbol{q},\boldsymbol{p})/\varepsilon}\bar{G}^\varepsilon_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{y})\Psi_0(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p} = 0. \tag{4.16}$$

Lemma 4.6. *For any d-vector function $\boldsymbol{v}(\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})$ such that each component is in $L^\infty(\mathbb{R}^d;\mathcal{S}(\mathbb{R}^d\times\Gamma^*))$*

$$\boldsymbol{v}(\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})\cdot(\boldsymbol{x}-\boldsymbol{Q}_n)\sim_n -\varepsilon\partial_{\boldsymbol{z}}\cdot(\boldsymbol{v}Z_n^{-1}), \tag{4.17}$$

and for any $d\times d$ matrix function $M(\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})$ such that each component is in $L^\infty(\mathbb{R}^d;\mathcal{S}(\mathbb{R}^d\times\Gamma^*))$

$$\begin{aligned} \operatorname{tr}\left(M(\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})(\boldsymbol{x}-\boldsymbol{Q}_n)^2\right) \sim_n &\varepsilon\operatorname{tr}\left(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n M Z_n^{-1}\right) - \varepsilon\operatorname{tr}\left(\partial_{\boldsymbol{z}}M(\boldsymbol{x}-\boldsymbol{Q}_n)Z_n^{-1} + M(\boldsymbol{x}-\boldsymbol{Q}_n)\partial_{\boldsymbol{z}}Z_n^{-1}\right) \\ =&\varepsilon\operatorname{tr}\left(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n M Z_n^{-1}\right) + \varepsilon^2\operatorname{tr}\left(\partial_{\boldsymbol{z}}\left(\partial_{\boldsymbol{z}}M(Z_n^{-1})^2\right) + \partial_{\boldsymbol{z}}\left(M\partial_{\boldsymbol{z}}Z_n^{-1}\right)Z_n^{-1}\right). \end{aligned} \tag{4.18}$$

Higher order terms can be obtained recursively. In general we have for any multi-index α that $|\alpha|\geq 3$,

$$(\boldsymbol{x}-\boldsymbol{Q}_n)^\alpha \sim_n \mathcal{O}\left(\varepsilon^{\left\lfloor\frac{|\alpha|+1}{2}\right\rfloor}\right). \tag{4.19}$$

Proof. The proof of lemma 4.6 is essentially the same as in Lemma 3 of [36] and thus is omitted here. □

We now substitute (4.14) into the Schrödinger equation. For this we first compute the time and space derivatives on $\psi^\varepsilon_{\mathrm{FGA},\infty}$:

$$\begin{aligned}\mathrm{i}\varepsilon\partial_t\psi^\varepsilon_{\mathrm{FGA},\infty} =& \frac{1}{(2\pi\varepsilon)^{3d/2}}\iint_\Omega \{i\varepsilon\partial_t b^\varepsilon - (\partial_t S_n - \boldsymbol{P}_n\cdot\partial_t\boldsymbol{Q}_n + (\partial_t\boldsymbol{P}_n - \mathrm{i}\partial_t\boldsymbol{Q}_n)\cdot(\boldsymbol{x}-\boldsymbol{Q}_n))\, b^\varepsilon\}\times\\ &\times G^\varepsilon_{\boldsymbol{Q}_n,\boldsymbol{P}_n} e^{\mathrm{i}S_n/\varepsilon}\left\langle G^\varepsilon_{\boldsymbol{q},\boldsymbol{p}} u_n(\boldsymbol{p},\cdot/\varepsilon),\psi_0\right\rangle \,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}.\end{aligned}\tag{4.20}$$

$$\begin{aligned}\tfrac12\varepsilon^2\Delta\psi^\varepsilon_{\mathrm{FGA},\infty} =& \frac{1}{(2\pi\varepsilon)^{3d/2}}\iint_\Omega \Big[-\frac12(-\mathrm{i}\nabla_{\boldsymbol{X}} + \boldsymbol{P}_n)^2 b^\varepsilon - (\nabla_{\boldsymbol{X}} b^\varepsilon + \mathrm{i}b^\varepsilon\boldsymbol{P}_n)\cdot(\boldsymbol{x}-\boldsymbol{Q}_n) +\\ &+\frac12 b^\varepsilon|\boldsymbol{x}-\boldsymbol{Q}_n|^2 - \frac12\varepsilon b^\varepsilon d\Big]\times\\ &\times G^\varepsilon_{\boldsymbol{Q}_n,\boldsymbol{P}_n} e^{\mathrm{i}S_n/\varepsilon}\left\langle G^\varepsilon_{\boldsymbol{q},\boldsymbol{p}} u_n(\boldsymbol{p},\cdot/\varepsilon),\psi_0\right\rangle \,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}.\end{aligned}\tag{4.21}$$

Hence, after rearranging terms, we arrive at

$$\begin{aligned}&\big(\mathrm{i}\varepsilon\partial_t + \frac12\varepsilon^2\Delta - V(\boldsymbol{X}) - U(\boldsymbol{x})\big)\psi^\varepsilon_{\mathrm{FGA},\infty} =\\ &= \frac{1}{(2\pi\varepsilon)^{3d/2}}\iint_\Omega \Big\{\Big[-\frac12(-\mathrm{i}\nabla_{\boldsymbol{X}} + \boldsymbol{P}_n)^2 - V(\boldsymbol{X}) - U(\boldsymbol{x}) - \partial_t S_n\Big]b^\varepsilon +\\ &\quad + \varepsilon\big(\mathrm{i}\partial_t b^\varepsilon - \frac12 b^\varepsilon d\big) - [(\nabla_{\boldsymbol{X}} b^\varepsilon + \mathrm{i}b^\varepsilon\boldsymbol{P}_n) + (\partial_t\boldsymbol{P}_n - \mathrm{i}\partial_t\boldsymbol{Q}_n)b^\varepsilon]\cdot(\boldsymbol{x}-\boldsymbol{Q}_n) +\\ &\quad + \frac12|\boldsymbol{x}-\boldsymbol{Q}_n|^2 b^\varepsilon + \boldsymbol{P}_n\cdot\partial_t\boldsymbol{Q}_n b^\varepsilon\Big\} G^\varepsilon_{\boldsymbol{Q}_n,\boldsymbol{P}_n} e^{\mathrm{i}S_n/\varepsilon}\left\langle G^\varepsilon_{\boldsymbol{q},\boldsymbol{p}} u_n(\boldsymbol{p},\cdot/\varepsilon),\psi_0\right\rangle \,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}.\end{aligned}\tag{4.22}$$

Define

$$\begin{aligned}f(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p}) = &\Big\{\Big[-\frac12(-\mathrm{i}\nabla_{\boldsymbol{X}} + \boldsymbol{P}_n)^2 - V(\boldsymbol{X}) - U(\boldsymbol{x}) - \partial_t S_n\Big]b^\varepsilon +\\ &+ \varepsilon\big(\mathrm{i}\partial_t b^\varepsilon - \frac12 b^\varepsilon d\big) - [(\nabla_{\boldsymbol{X}} b^\varepsilon + \mathrm{i}b^\varepsilon\boldsymbol{P}_n) + (\partial_t\boldsymbol{P}_n - \mathrm{i}\partial_t\boldsymbol{Q}_n)b^\varepsilon]\cdot(\boldsymbol{x}-\boldsymbol{Q}_n) +\\ &+ \frac12|\boldsymbol{x}-\boldsymbol{Q}_n|^2 b^\varepsilon + \boldsymbol{P}_n\cdot\partial_t\boldsymbol{Q}_n b^\varepsilon\Big\}\bar u_n(\boldsymbol{p},\boldsymbol{Y}),\end{aligned}\tag{4.23}$$

then we can write

$$\begin{aligned}&\big(\mathrm{i}\varepsilon\partial_t + \frac12\varepsilon^2\Delta - V(\boldsymbol{X}) - U(\boldsymbol{x})\big)\psi^\varepsilon_{\mathrm{FGA},\infty} =\\ &\qquad = \frac{1}{(2\pi\varepsilon)^{3d/2}}\iint_\Omega\int_{\mathbb{R}^d} f(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{p},\boldsymbol{q}) G^\varepsilon_{\boldsymbol{Q}_n,\boldsymbol{P}_n} e^{\mathrm{i}S_n/\varepsilon}\bar G^\varepsilon_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{y})\psi_0(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}.\end{aligned}\tag{4.24}$$

Applying Lemma 4.6 and adding and subtracting $U(\boldsymbol{Q}_n)$, we get

$$\begin{aligned}f \sim_n &\Big(-\tfrac12(-\mathrm{i}\nabla_{\boldsymbol{X}} + \boldsymbol{P}_n)^2 - V(\boldsymbol{X}) - (U(\boldsymbol{x}) - U(\boldsymbol{Q}_n)) - \partial_t S_n\Big) b^\varepsilon \bar u_n(\boldsymbol{p},\boldsymbol{Y})\\ &+ \varepsilon\big(\mathrm{i}\partial_t b^\varepsilon - \frac12 b^\varepsilon d\big)\bar u_n(\boldsymbol{p},\boldsymbol{Y})\\ &+ \varepsilon\partial_{\boldsymbol{z}}\Big([(\nabla_{\boldsymbol{X}} b^\varepsilon + \mathrm{i}b^\varepsilon\boldsymbol{P}_n) + (\partial_t\boldsymbol{P}_n - \mathrm{i}\partial_t\boldsymbol{Q}_n)b^\varepsilon]\,\bar u_n(\boldsymbol{p},\boldsymbol{Y})Z_n^{-1}\Big)\\ &+ \varepsilon\frac12 b^\varepsilon\,\mathrm{tr}\left[\partial_{\boldsymbol{z}}\boldsymbol{Q}_n Z_n^{-1}\right]\bar u_n(\boldsymbol{p},\boldsymbol{Y}) + \varepsilon^2\frac12\,\mathrm{tr}\left[\partial_{\boldsymbol{z}}\left(\partial_{\boldsymbol{z}}\left(b^\varepsilon\bar u_n(\boldsymbol{p},\boldsymbol{Y})Z_n^{-1}\right)Z_n^{-1}\right)\right]\\ &+ \boldsymbol{P}_n\cdot\partial_t\boldsymbol{Q}_n b^\varepsilon\bar u_n(\boldsymbol{p},\boldsymbol{Y}) - U(\boldsymbol{Q}_n) b^\varepsilon\bar u_n(\boldsymbol{p},\boldsymbol{Y})\end{aligned}\tag{4.25}$$

Use the Taylor expansion of $U(\boldsymbol{x})$ about $\boldsymbol{Q}_n$

$$(U(\boldsymbol{x}) - U(\boldsymbol{Q}_n)) = \nabla U(\boldsymbol{Q}_n)(\boldsymbol{x}-\boldsymbol{Q}_n) + \frac{1}{2!}\nabla^2 U(\boldsymbol{Q}_n)(\boldsymbol{x}-\boldsymbol{Q}_n)^2 + \frac{1}{3!}\nabla^3 U(\boldsymbol{Q}_n)(\boldsymbol{x}-\boldsymbol{Q}_n)^3 + \frac{1}{4!}\nabla^4 U(\boldsymbol{Q}_n)(\boldsymbol{x}-\boldsymbol{Q}_n)^4 + \sum_{|\alpha|=5} R_\alpha(\boldsymbol{x})(\boldsymbol{x}-\boldsymbol{Q}_n)^\alpha \tag{4.26}$$

with

$$R_\alpha(\boldsymbol{x}) = \frac{|\alpha|}{5!}\int_0^1 (1-\tau)^{|\alpha|-1}\partial^\alpha_{\boldsymbol{Q}_n} U(\boldsymbol{Q}_n + \tau(\boldsymbol{x}-\boldsymbol{Q}_n))d\tau. \tag{4.27}$$

From now on, let us denote the remainder term in (4.26) by $R(\boldsymbol{x},\boldsymbol{q},\boldsymbol{p})$.

Applying Lemma 4.6 again to (4.25) together with (4.26), we obtain

$$\begin{aligned} f \sim_n & \Big(-\frac{1}{2}(-\mathrm{i}\nabla_{\boldsymbol{X}} + \boldsymbol{P}_n)^2 - V(\boldsymbol{X}) - \partial_t S_n\Big) b^\varepsilon \bar{u}_n(\boldsymbol{p},\boldsymbol{Y}) \\ & + \boldsymbol{P}_n\cdot\partial_t \boldsymbol{Q}_n b^\varepsilon \bar{u}_n(\boldsymbol{p},\boldsymbol{Y}) - U(\boldsymbol{Q}_n) b^\varepsilon \bar{u}_n(\boldsymbol{p},\boldsymbol{Y}) \\ & + \varepsilon\Big(\mathrm{i}\partial_t b^\varepsilon - \frac{1}{2} b^\varepsilon d\Big)\bar{u}_n(\boldsymbol{p},\boldsymbol{Y}) + \varepsilon\partial_{\boldsymbol{z}}\left(\nabla U(\boldsymbol{Q}_n) b^\varepsilon \bar{u}_n(\boldsymbol{p},\boldsymbol{Y}) Z_n^{-1}\right) \\ & + \varepsilon\partial_{\boldsymbol{z}}\left(\left[(\nabla_{\boldsymbol{X}} b^\varepsilon + \mathrm{i} b^\varepsilon \boldsymbol{P}_n) + (\partial_t \boldsymbol{P}_n - \mathrm{i}\partial_t \boldsymbol{Q}_n) b^\varepsilon\right]\bar{u}_n(\boldsymbol{p},\boldsymbol{Y}) Z_n^{-1}\right) \\ & + \varepsilon\frac{1}{2!}\operatorname{tr}\left[\partial_{\boldsymbol{z}}\boldsymbol{Q}_n (I - \nabla^2 U(\boldsymbol{Q}_n)) b^\varepsilon \bar{u}_n(\boldsymbol{p},\boldsymbol{Y}) Z_n^{-1}\right] \\ & + \varepsilon^2\frac{1}{2!}\operatorname{tr}\left[\partial_{\boldsymbol{z}}(\partial_{\boldsymbol{z}}((I-\nabla^2 U(\boldsymbol{Q}_n)) b^\varepsilon \bar{u}_n(\boldsymbol{p},\boldsymbol{Y}) Z_n^{-1}) Z_n^{-1})\right] \\ & + \varepsilon^2\frac{2}{3!}\operatorname{tr}\left[\partial_{\boldsymbol{z}}(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n \nabla^3 U(\boldsymbol{Q}_n) b^\varepsilon \bar{u}_n(\boldsymbol{p},\boldsymbol{Y})(Z_n^{-1})^2)\right] \\ & + \varepsilon^2\frac{1}{3!}\operatorname{tr}\left[\partial_{\boldsymbol{z}}\boldsymbol{Q}_n \partial_{\boldsymbol{z}}(\nabla^3 U(\boldsymbol{Q}_n) b^\varepsilon \bar{u}_n(\boldsymbol{p},\boldsymbol{Y}) Z_n^{-1}) Z_n^{-1}\right] \\ & - \varepsilon^2\frac{3}{4!}\operatorname{tr}\left[(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n)^2 \nabla^4 U(\boldsymbol{Q}_n) b^\varepsilon \bar{u}_n(\boldsymbol{p},\boldsymbol{Y})(Z_n^{-1})^2\right] + R(\boldsymbol{x},\boldsymbol{q},\boldsymbol{p}) b^\varepsilon \bar{u}_{n,\boldsymbol{p}}(\boldsymbol{Y}). \end{aligned} \tag{4.28}$$

Let us define three operators L_0^n, L_1^n, and L_2^n acting on $\Phi = \Phi(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p})$ by

$$\begin{aligned} L_0^n(\Phi) := & \Big(-\frac{1}{2}(-\mathrm{i}\nabla_{\boldsymbol{X}} + \boldsymbol{P}_n)^2 - V(\boldsymbol{X}) - \partial_t S_n\Big)\Phi \\ & + \boldsymbol{P}_n\cdot\partial_t\boldsymbol{Q}_n\Phi - U(\boldsymbol{Q}_n)\Phi \\ = & \left(-H_{\boldsymbol{P}_n} + E_n(\boldsymbol{P}_n)\right)\Phi, \end{aligned} \tag{4.29}$$

$$\begin{aligned} L_1^n(\Phi) := & \Big(\mathrm{i}\partial_t\Phi - \frac{1}{2}\Phi d\Big) + \partial_{\boldsymbol{z}}\left(\nabla U(\boldsymbol{Q}_n)\Phi Z_n^{-1}\right) \\ & + \partial_{\boldsymbol{z}}\left(\left[(\nabla_{\boldsymbol{X}}\Phi + \mathrm{i}\Phi\boldsymbol{P}_n) + (\partial_t\boldsymbol{P}_n - \mathrm{i}\partial_t\boldsymbol{Q}_n)\Phi\right] Z_n^{-1}\right) \\ & + \frac{1}{2!}\operatorname{tr}\left[\partial_{\boldsymbol{z}}\boldsymbol{Q}_n(I - \nabla^2 U(\boldsymbol{Q}_n))\Phi Z_n^{-1}\right], \end{aligned} \tag{4.30}$$

and

$$\begin{aligned} L_2^n(\Phi) := & \frac{1}{2!}\operatorname{tr}\left[\partial_{\boldsymbol{z}}(\partial_{\boldsymbol{z}}((I-\nabla^2 U(\boldsymbol{Q}_n))\Phi Z_n^{-1}) Z_n^{-1})\right] \\ & + \frac{2}{3!}\operatorname{tr}\left[\partial_{\boldsymbol{z}}(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n\nabla^3 U(\boldsymbol{Q}_n)\Phi(Z_n^{-1})^2)\right] \\ & + \frac{1}{3!}\operatorname{tr}\left[\partial_{\boldsymbol{z}}\boldsymbol{Q}_n\partial_{\boldsymbol{z}}(\nabla^3 U(\boldsymbol{Q}_n)\Phi Z_n^{-1}) Z_n^{-1}\right] \\ & - \frac{3}{4!}\operatorname{tr}\left[(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n)^2\nabla^4 U(\boldsymbol{Q}_n)\Phi(Z_n^{-1})^2\right]. \end{aligned} \tag{4.31}$$

We thus arrive at

$$
\begin{aligned}
(4.32)\quad & \big(\mathrm{i}\varepsilon\partial_t + \tfrac{1}{2}\varepsilon^2\Delta - V(\boldsymbol{X}) - U(\boldsymbol{x})\big)\psi^{\varepsilon}_{\mathrm{FGA},\infty} \\
&= \frac{1}{(2\pi\varepsilon)^{3d/2}} \iint_{\Omega}\int_{\mathbb{R}^d} \big\{L_0^n(b^{\varepsilon}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})) + \varepsilon L_1^n(b^{\varepsilon}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})) \\
&\quad + \varepsilon^2 L_2^n(b^{\varepsilon}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})) + R(\boldsymbol{x},\boldsymbol{q},\boldsymbol{p}) b^{\varepsilon}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})\big\}\, G^{\varepsilon}_{\boldsymbol{Q}_n,\boldsymbol{P}_n} e^{\mathrm{i}S_n/\varepsilon} \bar{G}^{\varepsilon}_{\boldsymbol{q},\boldsymbol{p}}(\boldsymbol{y})\psi_0(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}.
\end{aligned}
$$

Note that by the choice $b_{n,0} = a_{n,0}u_n(\boldsymbol{P}_n,\boldsymbol{X})$, the $\mathcal{O}(1)$ term in the integrand on the right hand side of (4.32) vanishes as

$$
(4.33)\qquad L_0^n(a_{n,0}(t,\boldsymbol{q},\boldsymbol{p})u_n(\boldsymbol{p},\boldsymbol{X})) = a_{n,0}(t,\boldsymbol{q},\boldsymbol{p})\big(-H_{\boldsymbol{P}_n} + E_n(\boldsymbol{P}_n)\big)u_n(\boldsymbol{P}_n,\boldsymbol{X}) = 0
$$

for any $a_{n,0}$.

4.3.1. *Leading order term* $b_{n,0}$. To determine $a_{n,0}$, we set the order $\mathcal{O}(\varepsilon)$ term on the right hand side of (4.32) to zero and get

$$
(4.34)\qquad L_0^n(b_{n,1}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})) = -L_1^n(b_{n,0}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})).
$$

We multiply the equation by $\bar{u}_n(\boldsymbol{P}_n,\boldsymbol{X})$ and integrate over Γ; this gives

$$
(4.35)\qquad \partial_t a_{n,0} = \frac{1}{2}a_{n,0}\,\mathrm{tr}\left(\partial_{\boldsymbol{z}}\boldsymbol{P}_n(\nabla^2_{\boldsymbol{P}_n}E_n)Z_n^{-1}\right) - \mathrm{i}a_{n,0}\mathcal{A}(\boldsymbol{P}_n)\cdot\nabla_{\boldsymbol{Q}_n}U - \frac{\mathrm{i}}{2}a_{n,0}\,\mathrm{tr}(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n(\nabla^2_{\boldsymbol{Q}_n}U)Z_n^{-1}).
$$

Indeed, by integration, we get (index n is suppressed)

$$
\begin{aligned}
(4.36)\quad & \int_{\Gamma}\bar{u}_n(\boldsymbol{P}_n,\boldsymbol{X})\Big(-\tfrac{1}{2}(-\mathrm{i}\nabla_{\boldsymbol{X}}+\boldsymbol{P}_n)^2 - V(\boldsymbol{X}) - \partial_t S_n\Big)b_1\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})\,\mathrm{d}\boldsymbol{X} \\
&+ \int_{\Gamma}\Big\{\bar{u}_n(\boldsymbol{P}_n,\boldsymbol{X})\big(\mathrm{i}\partial_t b_0 - \frac{1}{2}b_0 d\big)\bar{u}_n(\boldsymbol{p},\boldsymbol{Y}) + \bar{u}_n(\boldsymbol{P}_n,\boldsymbol{X})\partial_{\boldsymbol{z}}\left(\nabla U(\boldsymbol{Q}_n)b_0\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})Z_n^{-1}\right) \\
&\quad + \bar{u}_n(\boldsymbol{P}_n,\boldsymbol{X})\partial_{\boldsymbol{z}}\Big([(\nabla_{\boldsymbol{X}}b_0 + \mathrm{i}b_0\boldsymbol{P}_n) + (\partial_t\boldsymbol{P}_n - \mathrm{i}\partial_t\boldsymbol{Q}_n)b_0]\,\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})Z_n^{-1}\Big) \\
&\quad + \bar{u}_n(\boldsymbol{P}_n,\boldsymbol{X})\frac{1}{2!}\,\mathrm{tr}\left[\partial_{\boldsymbol{z}}\boldsymbol{Q}_n(I - \nabla^2 U(\boldsymbol{Q}_n))b_0\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})Z_n^{-1}\right]\Big\}\,\mathrm{d}\boldsymbol{X} = 0.
\end{aligned}
$$

The perpendicular terms in the b_j's will now drop out and we can symplify this equation to

$$
\begin{aligned}
(4.37)\quad & -\left\langle u_n(\boldsymbol{P}_n,\boldsymbol{X}), \partial_{\boldsymbol{z}}\left([\mathrm{i}u_n(\boldsymbol{P}_n,\boldsymbol{X})\nabla_{\mathbf{P}_n}E_n - \nabla_{\boldsymbol{X}}u_n(\boldsymbol{P}_n,\boldsymbol{X}) - \mathrm{i}u_n(\boldsymbol{P}_n,\boldsymbol{X})\boldsymbol{P}_n]a_0\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})Z_n^{-1}\right)\right\rangle \\
&+ \Big(\mathrm{i}\partial_t a_0 - a_0\mathcal{A}(\boldsymbol{P}_n)\cdot\nabla_{\boldsymbol{Q}_n}U - \frac{d}{2}a_0\Big)\bar{u}_n(\boldsymbol{p},\boldsymbol{Y}) + \frac{1}{2}a_0\,\mathrm{tr}(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n(I - \nabla^2_{\boldsymbol{Q}_n}U)Z_n^{-1})\bar{u}_n(\boldsymbol{p},\boldsymbol{Y}) = 0.
\end{aligned}
$$

Using (2.11), we observe that

(4.38)

$$
\left\langle u_n(\boldsymbol{P}_n,\boldsymbol{X}), [\mathrm{i}u_n(\boldsymbol{P}_n,\boldsymbol{X})\nabla_{\boldsymbol{P}_n}E_n - \nabla_{\boldsymbol{X}}u_n(\boldsymbol{P}_n,\boldsymbol{X}) - \mathrm{i}u_n(\boldsymbol{P}_n,\boldsymbol{X})\boldsymbol{P}_n]\cdot\partial_z(a_0\bar{u}_n(\boldsymbol{P}_n,\boldsymbol{Y})Z_n^{-1})\right\rangle = 0.
$$

Hence, we arrive at

$$
\begin{aligned}
(4.39)\quad & a_0\,\mathrm{tr}\Big(\langle u_n(\boldsymbol{P}_n,\boldsymbol{X}), \partial_{\boldsymbol{z}}\cdot[\mathrm{i}u_n(\boldsymbol{P}_n,\boldsymbol{X})\nabla_{\boldsymbol{P}_n}E_n - \nabla_{\boldsymbol{X}}u_n(\boldsymbol{P}_n,\boldsymbol{X}) - \mathrm{i}u_n(\boldsymbol{P}_n,\boldsymbol{X})\boldsymbol{P}_n]\rangle\,Z_n^{-1}\Big) + \\
&+ \left(\mathrm{i}\partial_t a_0 - a_0\mathcal{A}(\boldsymbol{P}_n)\cdot\nabla_{\boldsymbol{Q}_n}U - \frac{d}{2}a_0\right) + \frac{1}{2}a_0\,\mathrm{tr}\big(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n(I - \nabla^2_{\boldsymbol{Q}_n}U)Z_n^{-1}\big) = 0.
\end{aligned}
$$

To further simplify the equation, observe that

$$
\begin{aligned}
&\Big\langle u_n(\boldsymbol{P}_n,\boldsymbol{X}), \partial_{\boldsymbol{z}}\cdot[\mathrm{i}u_n(\boldsymbol{P}_n,\boldsymbol{X})\nabla_{\boldsymbol{P}_n}E_n - \nabla_{\boldsymbol{X}}u_n(\boldsymbol{P}_n,\boldsymbol{X}) - \mathrm{i}u_n(\boldsymbol{P}_n,\boldsymbol{X})\boldsymbol{P}_n]\Big\rangle \\
&\quad= \mathrm{i}\left\langle u_n(\boldsymbol{P}_n,\boldsymbol{X}), \partial_{\boldsymbol{z}}u_n(\boldsymbol{P}_n,\boldsymbol{X})\right\rangle(\nabla_{\boldsymbol{P}_n}E_n - \boldsymbol{P}_n) - \left\langle u_n(\boldsymbol{P}_n,\boldsymbol{X}), \partial_{\boldsymbol{z}}\nabla_{\boldsymbol{X}}u_n(\boldsymbol{P}_n,\boldsymbol{X})\right\rangle \\
&\qquad + \mathrm{i}(\partial_{\boldsymbol{z}}\nabla_{\boldsymbol{P}_n}E_n - \partial_{\boldsymbol{z}}\boldsymbol{P}_n) \\
&\quad= \mathrm{i}\partial_{\boldsymbol{z}}\boldsymbol{P}_n\left\langle u_n(\boldsymbol{P}_n,\boldsymbol{X}), \partial_{\boldsymbol{P}_n}u_n(\boldsymbol{P}_n,\boldsymbol{X})\right\rangle(\nabla_{\boldsymbol{P}_n}E_n - \boldsymbol{P}_n) \\
&\qquad - \partial_{\boldsymbol{z}}\boldsymbol{P}_n\left\langle u_n(\boldsymbol{P}_n,\boldsymbol{X}), \nabla_{\boldsymbol{p}}\nabla_{\boldsymbol{X}}u_n(\boldsymbol{P}_n,\boldsymbol{X})\right\rangle_\Gamma + \mathrm{i}\partial_{\boldsymbol{z}}\boldsymbol{P}_n(\nabla^2_{\boldsymbol{P}_n}E_n - I) \\
&\quad\overset{(2.13)}{=} \frac{1}{2}\mathrm{i}\partial_{\boldsymbol{z}}\boldsymbol{P}_n(\nabla^2_{\boldsymbol{P}_n}E_n - I).
\end{aligned}
\tag{4.40}
$$

Putting this into (4.39), we have

$$
\begin{aligned}
&\frac{1}{2}\mathrm{i}a_0\,\mathrm{tr}\left(\partial_{\boldsymbol{z}}\boldsymbol{P}_n(I-\nabla^2_{\boldsymbol{P}_n}E_n)Z^{-1}\right) + \left(\mathrm{i}\partial_t a_0 - a_0\mathcal{A}(\boldsymbol{P}_n)\cdot\nabla_{\boldsymbol{Q}_n}U - \frac{d}{2}a_0\right) \\
&\qquad\qquad + \frac{1}{2}a_0\,\mathrm{tr}(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n(I-\nabla^2_{\boldsymbol{Q}_n}U)Z_n^{-1})] = 0.
\end{aligned}
\tag{4.41}
$$

We arrive at (4.35) finally by noting that

$$
\frac{1}{2}a\,\mathrm{tr}\left[\partial_{\boldsymbol{z}}\boldsymbol{Q}_n Z_n^{-1}\right] + \frac{\mathrm{i}}{2}a\,\mathrm{tr}\left[\partial_{\boldsymbol{z}}\boldsymbol{P}_n Z_n^{-1}\right] = \frac{1}{2}a\,\mathrm{tr}\left[Z_n Z_n^{-1}\right] = \frac{d}{2}a. \tag{4.42}
$$

4.3.2. *Next order term $b_{n,1}$.* To characterize $b_{n,1}$, we set the order $\mathcal{O}(\varepsilon^2)$ term in (4.32) to zero, we have

$$
\int_\Gamma \bar{u}_n(\boldsymbol{P}_n,\boldsymbol{X})\left(L_0^n(b_{n,2}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})) + L_1^n(b_{n,1}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})) + L_2^n(b_{n,0}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y}))\right)d\boldsymbol{X} = 0. \tag{4.43}
$$

Let us first derive the equation for a_1. We start with (4.43) written in expanded form

(4.44)

$$
\begin{aligned}
&\int_\Gamma \bar{u}_n(\boldsymbol{P}_n,\boldsymbol{X})\bigg\{\frac{1}{2!}\,\mathrm{tr}\left[\partial_{\boldsymbol{z}}(\partial_{\boldsymbol{z}}((I-\nabla^2U(\boldsymbol{Q}_n))b_0\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})Z_n^{-1})Z_n^{-1})\right] \\
&\qquad + \frac{2}{3!}\,\mathrm{tr}\left[\partial_{\boldsymbol{z}}(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n\nabla^3U(\boldsymbol{Q}_n)b_0\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})(Z_n^{-1})^2)\right] \\
&\qquad + \frac{1}{3!}\,\mathrm{tr}\left[\partial_{\boldsymbol{z}}\boldsymbol{Q}_n\partial_{\boldsymbol{z}}(\nabla^3U(\boldsymbol{Q}_n)b_0\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})Z_n^{-1})Z_n^{-1}\right] - \frac{3}{4!}\,\mathrm{tr}\left[(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n)^2\nabla^4U(\boldsymbol{Q}_n)b_0\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})(Z_n^{-1})^2\right] \\
&\qquad + \left(\mathrm{i}\partial_t b_1 - \frac{1}{2}b_1 d\right)\bar{u}_n(\boldsymbol{p},\boldsymbol{Y}) + \partial_{\boldsymbol{z}}\left(\nabla U(\boldsymbol{Q}_n)b_1\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})Z_n^{-1}\right) \\
&\qquad + \partial_{\boldsymbol{z}}\left([(\nabla_{\boldsymbol{X}}b_1 + \mathrm{i}b_1\boldsymbol{P}_n) + (\partial_t\boldsymbol{P}_n - \mathrm{i}\partial_t\boldsymbol{Q}_n)b_1]\,\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})Z_n^{-1}\right) \\
&\qquad + \frac{1}{2!}\,\mathrm{tr}\left[\partial_{\boldsymbol{z}}\boldsymbol{Q}_n(I-\nabla^2U(\boldsymbol{Q}_n))b_1\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})Z_n^{-1}\right] + \left(-H_{\boldsymbol{P}_n} + E(\boldsymbol{P}_n)\right)b_2\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})\bigg\}\,d\boldsymbol{X} = 0.
\end{aligned}
$$

Making use of the Hamiltonian flow (3.2) and the identity (4.38), we arrive at

$$
\begin{aligned}
&-\mathrm{tr}\Big(\left\langle u_{\boldsymbol{P}_n}, \partial_{\boldsymbol{z}}\cdot[u(\mathrm{i}\nabla E_n(\boldsymbol{P}_n)) - \nabla_{\boldsymbol{X}}u - \mathrm{i}u\boldsymbol{P}_n](a_1)\right\rangle Z_n^{-1}\Big) \\
&\qquad + \left(\mathrm{i}\partial_t a_1 - a_1\mathcal{A}(\boldsymbol{P}_n)\cdot\nabla_{\boldsymbol{Q}_n}U - \frac{d}{2}a_1\right) + a_0\frac{1}{2}\,\mathrm{tr}\Big(\partial_{\boldsymbol{z}}(\partial_{\boldsymbol{z}}[(I-\nabla^2_{\boldsymbol{Q}_n}U)Z_n^{-1}]Z_n^{-1})\Big) \\
&\qquad + a_1\frac{1}{2}\,\mathrm{tr}\Big(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n(I-\nabla^2_{\boldsymbol{Q}_n}U)Z_n^{-1}\Big) + \frac{2}{3!}a_0\,\mathrm{tr}\Big(\partial_{\boldsymbol{z}}(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n\nabla^3_{\boldsymbol{Q}_n}U(Z_n^{-1})^2)\Big) \\
&\qquad + \frac{1}{3!}a_0\,\mathrm{tr}\Big(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n\partial_{\boldsymbol{z}}(\nabla^3_{\boldsymbol{Q}_n}UZ_n^{-1})Z_n^{-1}\Big) - \frac{3}{4!}a_0\,\mathrm{tr}\Big((\partial_{\boldsymbol{z}}\boldsymbol{Q}_n)^2\nabla^4_{\boldsymbol{Q}_n}U(Z_n^{-1})^2\Big) = 0.
\end{aligned}
\tag{4.45}
$$

Then using (4.40) and (4.42), upon simplification we obtain the equation for $a_{n,1}$

$$\begin{aligned}\partial_t a_{n,1} =& -\mathrm{i}a_{n,1}\mathcal{A}(\boldsymbol{P}_n)\cdot\nabla_{\boldsymbol{Q}_n}U+\frac{1}{2}a_{n,1}\operatorname{tr}\left(\partial_{\boldsymbol{z}}\boldsymbol{P}_n(\nabla^2_{\boldsymbol{P}_n}E_n)Z_n^{-1}\right)-\frac{\mathrm{i}}{2}a_{n,1}\operatorname{tr}\left(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n(\nabla^2_{\boldsymbol{Q}_n}U)Z_n^{-1}\right)\\ &+\frac{\mathrm{i}}{2}a_{n,0}\operatorname{tr}\left(\partial_{\boldsymbol{z}}(\partial_{\boldsymbol{z}}[(I-\nabla^2_{\boldsymbol{Q}_n}U)Z_n^{-1}]Z_n^{-1})\right)+\frac{2\mathrm{i}}{3!}a_{n,0}\operatorname{tr}\left(\partial_{\boldsymbol{z}}(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n\nabla^3_{\boldsymbol{Q}_n}U(Z_n^{-1})^2)\right)\\ &+\frac{\mathrm{i}}{3!}a_{n,0}\operatorname{tr}\left(\partial_{\boldsymbol{z}}\boldsymbol{Q}_n\partial_{\boldsymbol{z}}(\nabla^3_{\boldsymbol{Q}_n}UZ_n^{-1})Z_n^{-1}\right)-\frac{3\mathrm{i}}{4!}a_{n,0}\operatorname{tr}\left((\partial_{\boldsymbol{z}}\boldsymbol{Q}_n)^2\nabla^4_{\boldsymbol{Q}_n}U(Z_n^{-1})^2\right).\end{aligned}\tag{4.46}$$

Define the operator $\mathcal{Q}=\mathrm{Id}-\Pi_n$ where Π_n is the projection operator onto the nth Bloch wave. $b^{\perp}_{n,1}$ satisfies $\Pi_n b^{\perp}_{n,1}=\left\langle u_n(\boldsymbol{P}_n,\boldsymbol{x}),b^{\perp}_{n,1}\right\rangle=0$, and is hence determined by applying $\mathcal{Q}$ to $L_0^n(b_{n,1}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y}))=-L_1^n(b_{n,0}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y}))$. We obtain

$$b^{\perp}_{n,1}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})=-\left(L_0^n\right)^{-1}\mathcal{Q}\left(L_1^n(b_{n,0}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y}))\right).\tag{4.47}$$

Note that the inverse of the operator L_0^n can be defined on its range.

Thus, we have obtained the equations for $a_{n,0}$ (4.35), $a_{n,1}$ (4.46), and $b^{\perp}_{n,1}$ (4.47). This can be continued to higher orders. Let us summarize the estimate of these terms in the following propositions.

Proposition 4.7. *For each $k\in\mathbb{N}$, the amplitudes $a_{n,0}$ and $a_{n,1}$, given by* (4.35) *and* (4.46) *satisfy*

$$\sup_{t\in[0,T]}M_k[a_{n,0}]<\infty,\qquad \textit{and}\qquad \sup_{t\in[0,T]}M_k[a_{n,1}]<\infty.\tag{4.48}$$

Proof. By (4.2), (4.3) and (4.4), we see that the right hand side of (4.35) and (4.46) are bounded by some constants independent of $\boldsymbol{q}$ and $\boldsymbol{p}$ times $a_{n,0}$ and $a_{n,1}$, respectively. An application of Gronwall's inequality yields the result. □

Proposition 4.8. *For each $k\in\mathbb{N}$ we have that*

$$\sup_{t\in[0,T]}M_k[b^{\perp}_{n,1}\bar{u}_n(\boldsymbol{P}_n,\boldsymbol{Y})]<\infty.\tag{4.49}$$

Proof. The equation for $b^{\perp}_{n,1}$ is given by equation (4.47). We thus obtain a bound by using the spectrum of L_0^n. We can write

$$(L_0^n)^{-1}(\Phi)=\sum_{m\neq n}\frac{\langle u_m(\boldsymbol{P}_m,\cdot),\Phi(\cdot,\boldsymbol{Y},\boldsymbol{q},\boldsymbol{p})\rangle_{L^2(\Gamma)}\,u_m(\boldsymbol{P}_m,\boldsymbol{X})}{E_n(\boldsymbol{P}_n)-E_m(\boldsymbol{P}_m)}.\tag{4.50}$$

Let $g=\min_{\boldsymbol{\xi}\in[-\pi,\pi]^d}\{|E_n(\boldsymbol{\xi})-E_{n-1}(\boldsymbol{\xi})|,|E_n(\boldsymbol{\xi})-E_{n+1}(\boldsymbol{\xi})|\}$. Then for each $k\in\mathbb{N}$, we obtain

$$\begin{aligned}M_k[b^{\perp}_{n,1}\bar{u}_n(\boldsymbol{P}_n,\boldsymbol{Y})]&\le M_k\left[\frac{1}{g}\sum_{m\neq n}\langle u_m(\boldsymbol{P}_m,\cdot),b_{n,0}(t,\cdot,\boldsymbol{q},\boldsymbol{p})\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})\rangle_{L^2(\Gamma)}\,u_n(\boldsymbol{P}_n,\boldsymbol{X})\right]\\ &=M_k\left[\frac{\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})}{g}\sum_{m\neq n}a_{n,0}(t,\boldsymbol{q},\boldsymbol{p})\,\langle u_m(\boldsymbol{P}_m,\cdot),u_n(\boldsymbol{P}_n,\cdot)\rangle_{L^2(\Gamma)}\,u_n(\boldsymbol{P}_n,\boldsymbol{X})\right].\end{aligned}\tag{4.51}$$

Hence, by Propositions 4.4 and 4.7, it suffices to control

$$M_k\Big[\sum_{m\neq n}\langle u_m(\boldsymbol{P}_m,\boldsymbol{X}),u_n(\boldsymbol{P}_n,\boldsymbol{X})\rangle_{L^2(\Gamma)}\Big].\tag{4.52}$$

Since $\int_\Gamma|u_n(\boldsymbol{\xi},\boldsymbol{x})|^2d\boldsymbol{x}=1$, Bessel's inequality implies that the above is finite. □

4.4. **Proof of Theorem 3.1.** We will need the following estimate, which is proved in [10, Lemma 2.8].

Lemma 4.9. *Suppose $H(\varepsilon)$ is a family of self-adjoint operators for $\varepsilon > 0$. Suppose $\psi(t,\varepsilon)$ belongs to the domain of $H(\varepsilon)$, is continuously differentiable in t and approximately solves the Schrodinger equation in the sense that*

$$\mathrm{i}\varepsilon\frac{\partial\psi}{\partial t}(t,\varepsilon) = H(\varepsilon)\psi(t,\varepsilon) + \zeta(t,\varepsilon), \tag{4.53}$$

where $\zeta(t,\varepsilon)$ satisfies

$$||\zeta(t,\varepsilon)|| \le \mu(t,\varepsilon). \tag{4.54}$$

Then,

$$e^{-\mathrm{i}tH(\varepsilon)/\varepsilon}\psi(0,\varepsilon) - \psi(t,\varepsilon) \le \varepsilon^{-1}\int_0^t \mu(s,\varepsilon)ds. \tag{4.55}$$

Moreover, for the Fourier integral operator, we have

Lemma 4.10. *If, for fixed $\boldsymbol{x},\boldsymbol{y} \in \mathbb{R}^d$, $u(\boldsymbol{x},\boldsymbol{y},\boldsymbol{q},\boldsymbol{p}) \in L^\infty(\Omega;\mathbb{C})$, for each $n \in \mathbb{N}$ and any t, $\mathcal{I}^\varepsilon(u)$ can be extended to a linear bounded operator on $L^2(\mathbb{R}^d,\mathbb{C})$, and we have*

$$||\mathcal{I}(u)||_{\mathscr{L}(L^2(\mathbb{R}^d;\mathbb{C}))} \le ||u||_{L^\infty(\mathbb{R}^{2d};\mathbb{C})}. \tag{4.56}$$

Proof. The proof of lemma 4.10 is essentially the same as Proposition 3.7 in [23] and thus is omitted here. □

We are now ready to prove Theorem 3.1.

Proof of Theorem 3.1. Computing $\mathrm{i}\varepsilon\frac{\partial}{\partial t} + \frac{1}{2}\varepsilon^2\nabla^2 - V(\boldsymbol{X}) - U(\boldsymbol{x})$ applied to $\mathcal{I}^\varepsilon\left(b_n^{\varepsilon,1}(t,\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{q},\boldsymbol{p})\bar{u}_n(\boldsymbol{p},\frac{\boldsymbol{y}}{\varepsilon})\right)$, we obtain

$$\left(\mathrm{i}\varepsilon\frac{\mathrm{d}}{\mathrm{d}t} + \frac{1}{2}\varepsilon^2\nabla^2 - V(\boldsymbol{X}) - U(\boldsymbol{x})\right)\mathcal{I}^\varepsilon\left(b_n^{\varepsilon,1}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})\right) = \mathcal{I}^\varepsilon\left(\sum_{j=0}^{1}\varepsilon^j v_{n,j}\right) + \varepsilon^2\mathcal{I}^\varepsilon\left(v_{n,2}^\varepsilon\right). \tag{4.57}$$

The expressions for $v_{n,0}$, $v_{n,1}$, and $v_{n,2}$ follows from (4.32) by expanding b^ε and the linearity of L_0^n, L_1^n, and L_2^n. By equations (4.33) and (4.34), $v_{n,0}$ and $v_{n,1}$ vanish. The remaining term

$$v_{n,2}^\varepsilon = L_2^n(b_n^{\varepsilon,1}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y})) + R(\boldsymbol{x},\boldsymbol{q},\boldsymbol{p})b_n^{\varepsilon,1}\bar{u}_n(\boldsymbol{p},\boldsymbol{Y}). \tag{4.58}$$

satisfies $M_k[v_{n,2}^\varepsilon] < \infty$ by Propositions 4.3, 4.7, and 4.8. Finally, applying Lemma 4.10 and Lemma 4.9 we obtain the inequality in Theorem 3.1. □

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