SIAM J. APPL. MATH.
Vol. 85, No. 1, pp. 314–340

RADIATIVE TRANSPORT IN A PERIODIC STRUCTURE WITH BAND CROSSINGS*

KUNLUN QI†, LI WANG†, AND ALEXANDER B. WATSON†

Abstract. We use the Wigner transformation and asymptotic analysis to systematically derive the semiclassical model for the Schrödinger equation in arbitrary spatial dimensions, with any periodic structure. Our particular emphasis lies in addressing the *diabatic* effect, i.e., the impact of Bloch band crossings. We consider both deterministic and random scenarios. In the former case, we derive a coupled Liouville system, revealing lower-order interactions among different Bloch bands. In the latter case, a coupled system of radiative transport equations emerges, with the scattering cross section induced by the random inhomogeneities. As a specific application, we deduce the effective dynamics of a wave packet in graphene with randomness.

Key words. semiclassical limit, Dirac equation, Wigner transform, Bloch theory, band crossing Schrödinger equation, waves in random media, radiative transport equation

MSC codes. 82C70, 35Q99, 35R60, 74A40, 74E05, 74Q10

DOI. 10.1137/24M1638082

1. Introduction.

The Schrödinger equation, serving as a model that describes the evolution of the quantum state of a physical system, such as an electron, over time, has found widespread application in solid-state physics. The equation is given by

$$\mathrm{i}\partial_t \phi(t,\mathbf{x}) + \frac{1}{2}\Delta\phi(t,\mathbf{x}) - V(\mathbf{x})\,\phi(t,\mathbf{x}) = 0, \quad t \in \mathbb{R}_+, \quad \mathbf{x} \in \mathbb{R}^d, \tag{1.1}$$

where $\phi(t,\mathbf{x})$ represents the complex-valued wave function. When the material displays a certain lattice structure, characterized by the periodicity in V (i.e., $V(\mathbf{x}+\boldsymbol{\nu}) = V(\mathbf{x})$ for any $\mathbf{x}$ in $\mathbb{R}^d$ and $\boldsymbol{\nu}$ being the lattice vector), Floquet–Bloch theory offers insight into the energy band structures of the material (elaborated in section 2.1). The interaction of these bands determines the *adiabatic* and *diabatic* behavior of the quantum system, depending on whether the bands intersect.

The latter scenario is particularly evident in structures with honeycomb lattice symmetry, such as graphene, a two-dimensional material composed of a single layer of carbon atoms [38]. Indeed, the energy dispersion surfaces of graphene reveal conical singularities at the intersections of the valence and conduction bands [19, 20, 9]. These singularities, termed *Dirac points,* form cone-like shapes centered at the vertices of the Brillouin zone, playing a pivotal role in its remarkable electronic and mechanical properties [37]. Graphene has attracted renewed attention in recent years since the observation that magic angle twisted bilayer graphene, i.e., two layers of graphene, stacked with a relative twist $\approx 1^\circ$, displays signs of unconventional superconductivity [11, 13, 12].

*Received by the editors February 8, 2024; accepted for publication (in revised form) November 7, 2024; published electronically February 11, 2025.
https://doi.org/10.1137/24M1638082
Funding: The work of the second author was partially supported by NSF grant DMS-1846854. The work of the third author was supported in part by NSF grants DMREF 1922165 and DMS 2406981.
†School of Mathematics, University of Minnesota–Twin Cities, Minneapolis, MN 55455 USA (kqi@umn.edu, liwang@umn.edu, abwatson@umn.edu).

When the initial data of (1.1) is concentrated at the Dirac points, Fefferman and Weinstein have demonstrated that the solution to (1.1) can be expressed as the superposition of Floquet–Bloch states with modulated amplitudes. These amplitudes adhere to the Dirac equations [20]. Consequently, an intriguing question arises: In the presence of material perturbations, such as impurities, what impact will it have on the Dirac equations?

To tackle this problem, rather than directly modifying the Dirac equations, we opt for a different approach by revisiting the Schrödinger equation and introducing a random potential to model the perturbation. Instead of following the derivation in [20], we consider a different scenario by incorporating a semiclassical scaling into the Schrödinger equation. This scaling facilitates the treatment of randomness. Specifically, under this scaling, (1.1) is rewritten into

$$\mathrm{i}\varepsilon\partial_t\phi_\varepsilon + \frac{\varepsilon^2}{2}\Delta_{\mathbf{x}}\phi_\varepsilon - V\left(\frac{\mathbf{x}}{\varepsilon}\right)\phi_\varepsilon - \sqrt{\varepsilon}N\left(\frac{\mathbf{x}}{\varepsilon}\right)\phi_\varepsilon = 0, \tag{1.2}$$

where ε is the rescaled Planck constant, and N denotes the random potential. The fundamental question now becomes, what is the semiclassical limit (i.e., $\varepsilon \downarrow 0$) of (1.2) in the presence of band crossings?

The primary tool we utilize here is the Wigner transform, which lifts the wave function from physical space to phase space by adding the dependence on quasi-momenta, and therefore bears a close analogy to the classical mechanics [45]. When both V and N are absent in (1.2), the semiclassical limit yields the Liouville equation. This result is rigorously established by Gérard in [24], and subsequently confirmed by Lions and Paul in [34], and Markowich and Mauser in [35]. When a periodic function V exists, Markowich, Mauser, and Poupaud in [36] have rigorously demonstrated that, following the approach outlined in [34], provided the bands are well-separated, the semiclassical limit remains the Liouville equation traversing each band. This result has been significantly expanded upon by Bechouche, Mauser, and Poupaud in [6], including both periodic and nonperiodic potentials, as well as the homogenization limit. There, a variation of the Wigner transform known as the Wigner–Bloch series has been introduced to handle the density matrices associated with two energy bands. All these works focus on the adiabatic dynamics.

To account for the diabatic dynamics, the well-known Landau–Zener formula quantifies the probability of a transition occurring between two energy levels [31, 47]. It has since then been extensively studied in the context of the surface hopping method, beyond the Born–Oppenheimer approximation. We refer the readers to analytical works in [27, 23, 21, 33, 32, 22, 14, 44] and computational studies in [30, 15, 16]. We mention in particular Chai, Jin, and Li in [14] who derived the semiclassical limit in the form of a coupled Liouville equation near band crossing points in one dimension.

In the presence of randomness, a radiative transport-type equation is anticipated in the semiclassical limit. This was initially identified by Spohn in [42], where he rigorously derived such a limit for time-dependent Gaussian random impurities. However, his result is limited to short times. Subsequently, Ho, Landau, and Wilkins refined Spohn's work by considering higher-order corrections in [28]. Erdös and Yau further extended these findings to include general initial conditions and removed the restriction on the smallness of time in [17]. Extensions of these findings to more general types of waves in random media, such as those described by hyperbolic systems, can be found in the work of Ryzhik, Papanicolaou, and Keller [40]. Further extensions, including the incorporation of periodic structures, are addressed by Bal et al. in [3], while the addition of nonlinear terms is investigated by Fannjiang, Jin, and Papanicolaou [18]. A rigorous derivation of the radiative transport limit of the

Schrödinger equation is established by Bal, Papanicolaou, and Ryzhik in [5], assuming time-dependent randomness and utilizing the concept of martingales. More recently, the inclusion of randomness in the Dirac equation has been explored by Bal, Gu, and Pinaud [4].

Building upon previous discoveries, in this work, we combine the techniques of the Wigner transform for handling semiclassical scaling and randomness with Floquet–Bloch theory to address periodicity. Our goal is to derive a coupled system describing energy propagation in the semiclassical limit, accounting both for the coupling between bands at band crossings, and for coupling between distinct wave vectors induced by randomness.

The results of this paper are as follows. In the absence of randomness, the semiclassical limit of (1.2) in the vicinity of the crossing point is a system of Liouville equations, reminiscent of the Dirac system of [20], with an additional relaxation-type source term; see (3.16). This term vanishes at the crossing point, thereby reducing the system to the homogeneous case. Here, we generalize the results of Chai, Jin, and Li [14] to higher dimensions. In the presence of randomness, an additional integral term emerges, reminiscent of the collision term in the radiative transport equation; see (4.15). This term describes the coupling between distinct wave vectors with the same energy. Here, we generalize the results of Balet al. [3], whose methods do not immediately extend to the case where bands have nonconstant multiplicities because of band crossings, as occurs in graphene at "Dirac points." To our knowledge, the models (4.16), (5.2), and (5.3)–(5.4) of the dynamics of electrons in materials with band crossings in the presence of randomness, modeled by (1.2), are original to the present work. The main difficulty in deriving these models is to address the subtle effect where band crossings not only affect the dynamics for quasi-momenta precisely at the crossing point, but also within an ε-dependent neighborhood of the crossing point. Within this neighborhood, the effects of the band crossing are of order 1 for quasi-momenta. The size of this neighborhood is ε-dependent and varies according to the precise form of the bands near the crossing point; see the discussions in sections 3.2, 4, 5, and Appendix C.

The rest of the paper is organized as follows. In the next section, we review some preliminary results concerning the Schrödinger equation with periodic potential, its associated Bloch theory, and the Wigner transform. Section 3 focuses on scenarios without randomness, where we derive a coupled Liouville system featuring a relaxation-type source term to account for band crossing effects. In section 4, we extend our analysis by introducing random perturbations, leading to the derivation of a coupled radiative transport system. The results are then applied to the honeycomb structure in section 5, where we elucidate the effective dynamics of wave packets in graphene with randomness. Finally, the paper is concluded in section 6.

2. Preliminaries.

2.1. The Floquet–Bloch theory. Letting $\{\mathbf{e}_1, \dots, \mathbf{e}_d\}$ be a basis in $\mathbb{R}^d$, we define a periodic lattice Λ as

$$\Lambda \stackrel{\text{def}}{=} \left\{ \sum_{j=1}^{d} m_j \mathbf{e}_j \,\Big|\, m_j \in \mathbb{Z},\, j = 1, \dots, d \right\}.$$

Then its dual lattice, denoted by Λ^*, is defined as

$$\Lambda^* \stackrel{\text{def}}{=} \left\{ \sum_{l=1}^{d} m_l \mathbf{e}^l \,\Big|\, m_l \in \mathbb{Z},\, l = 1, \dots, d \right\},$$

where $\mathbf{e}^l$ is the dual basis of $\mathbf{e}_j$ in the sense that

$$(\mathbf{e}_j \cdot \mathbf{e}^l) = 2\pi\delta_{jl}.$$

Additionally, we define the fundamental cell of Λ as $\mathcal{C}$,

$$\mathcal{C} \stackrel{\text{def}}{=} \left\{ \sum_{j=1}^{d} \theta_j \mathbf{e}_j \,\middle|\, 0 \le \theta_j < 1,\, j = 1, \ldots, d \right\},$$

and the Brillouin zone as $\mathcal{B}$,

$$\mathcal{B} \stackrel{\text{def}}{=} \left\{ \sum_{l=1}^{d} \theta_l \mathbf{e}^l \,\middle|\, 0 \le \theta_l < 1,\, l = 1, \ldots, d \right\}.$$

Throughout this paper, we will consider the real-valued potential function $V(\mathbf{x})$ with Λ periodicity, i.e.,

$$V(\mathbf{x} + \boldsymbol{\nu}) = V(\mathbf{x}) \quad \forall \mathbf{x} \in \mathbb{R}^d, \quad \boldsymbol{\nu} \in \Lambda.$$

Denote

$$H_V \stackrel{\text{def}}{=} -\frac{1}{2}\Delta_{\mathbf{x}} + V(\mathbf{x}).$$

For $\mathbf{k} \in \mathbb{R}^d$, we can consider the *Bloch* eigenvalue problem

$$\begin{cases} H_V \Psi(\mathbf{x}, \mathbf{k}) = E(\mathbf{k}) \Psi(\mathbf{x}, \mathbf{k}), \\ \Psi(\mathbf{x} + \boldsymbol{\nu}, \mathbf{k}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\boldsymbol{\nu}} \Psi(\mathbf{x}, \mathbf{k}) \quad \forall \boldsymbol{\nu} \in \Lambda, \\ \dfrac{\partial \Psi(\mathbf{x} + \boldsymbol{\nu}, \mathbf{k})}{\partial x_j} = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\boldsymbol{\nu}} \dfrac{\partial \Psi(\mathbf{x}, \mathbf{k})}{\partial x_j} \quad \forall \boldsymbol{\nu} \in \Lambda, \quad j = 1, \ldots, d. \end{cases} \tag{2.1}$$

We now summarize the essential properties of this eigenvalue problem. For more details, see [8, 39, 46].

(i) For each $\mathbf{k}$, the eigenvalue problem (2.1) is self-adjoint with compact resolvent. Hence, it has a real and discrete spectrum which can be ordered with the multiplicity

$$E_1(\mathbf{k}) \le E_2(\mathbf{k}) \le \cdots \le E_m(\mathbf{k}) \le \cdots \quad \text{with} \quad E_m(\mathbf{k}) \to \infty \quad \text{as } m \to \infty.$$

The associated Bloch eigenfunctions $\Psi_m(\mathbf{x}, \mathbf{k})$ form a complete orthonormal basis in $L^2(\mathcal{C})$ with

$$\frac{1}{|\mathcal{C}|} \int_{\mathcal{C}} \Psi_m(\mathbf{x}, \mathbf{k}) \, \overline{\Psi_j(\mathbf{x}, \mathbf{k})} \, \mathrm{d}\mathbf{x} = \delta_{mj}.$$

Here δ_{mj} is the Kronecker delta function.

(ii) The eigenvalue problem (2.1) is invariant under replacement of $\mathbf{k}$ by $\mathbf{k} + \boldsymbol{\mu}$ for $\boldsymbol{\mu} \in \Lambda^*$. Therefore it suffices to consider $\mathbf{k} \in \mathcal{B}$, and that the eigenvalue band functions $E_m(\mathbf{k})$ and associated eigenfunctions are both Λ^*-periodic functions of $\mathbf{k}$.

(iii) We identify $\Psi_m(\mathbf{x},\mathbf{k})$ with its pseudoperiodic extension from $\mathbf{x}\in\mathcal{C}$ to $\mathbf{x}\in\mathbb{R}^d$ by the boundary condition in $\mathbf{x}$ in (2.1). Then for any function $\phi(\mathbf{x})\in L^2(\mathbb{R}^d)$, we define its Bloch transform as

$$\tilde{\phi}_m(\mathbf{k}) = \int_{\mathbb{R}^d} \phi(\mathbf{x})\overline{\Psi_m(\mathbf{x},\mathbf{k})}\,\mathrm{d}\mathbf{x}, \tag{2.2}$$

then $\tilde{\phi}_m(\mathbf{k})$ possesses the following properties [3, p. 484]:

– For $\mathbf{x}\in\mathbb{R}^d$, one has the following Bloch decomposition of $\phi(\mathbf{x})\in L^2(\mathbb{R}^d)$,

$$\phi(\mathbf{x}) = \frac{1}{|\mathcal{B}|}\sum_{m=1}^{\infty}\int_{\mathcal{B}} \tilde{\phi}_m(\mathbf{k})\Psi_m(\mathbf{x},\mathbf{k})\,\mathrm{d}\mathbf{k}. \tag{2.3}$$

– For $\phi(\mathbf{x}),\psi(\mathbf{x})\in L^2(\mathbb{R}^d)$,

$$\int_{\mathbb{R}^d} \phi(\mathbf{x})\overline{\psi(\mathbf{x})}\,\mathrm{d}\mathbf{x} = \frac{1}{|\mathcal{B}|}\sum_{m=1}^{\infty}\int_{\mathcal{B}} \tilde{\phi}_m(\mathbf{k})\overline{\tilde{\psi}_m(\mathbf{k})}\,\mathrm{d}\mathbf{k}.$$

– The mapping $\phi\mapsto\tilde{\phi}$ is one to one and onto from $L^2(\mathbb{R}^d)\mapsto\oplus_m L^2(\mathcal{B})$.

(iv) Following from (2.2) and (2.3), we can deduce additional orthogonality conditions

$$\frac{1}{|\mathcal{B}|}\sum_{m=1}^{\infty}\int_{\mathcal{B}} \Psi_m(\mathbf{x},\mathbf{k}),\overline{\Psi_m(\mathbf{y},\mathbf{k})}\,\mathrm{d}\mathbf{k} = \delta(\mathbf{y}-\mathbf{x})$$

and

$$\frac{1}{|\mathcal{B}|}\int_{\mathbb{R}^d} \Psi_j(\mathbf{x},\mathbf{k}),\overline{\Psi_m(\mathbf{x},\tilde{\mathbf{k}})}\,\mathrm{d}\mathbf{x} = \delta_{jm}\delta_{\mathrm{per}}(\mathbf{k}-\tilde{\mathbf{k}}), \tag{2.4}$$

where δ_{mj} is the Kronecker delta, and δ_{per} is defined in the sense that

$$\forall\,\varphi(\mathbf{k})\in C^\infty(\mathcal{B}),\quad \varphi(\mathbf{k}) = \int_{\mathcal{B}} \varphi(\tilde{\mathbf{k}})\delta_{\mathrm{per}}(\mathbf{k}-\tilde{\mathbf{k}})\,\mathrm{d}\tilde{\mathbf{k}}.$$

2.2. The Wigner transform. We now examine the Schrödinger equation in the semiclassical scaling and introduce the Wigner transform, a crucial tool in our subsequent derivation.

The semiclassical scaling of (1.1) with initial condition $\phi(t=0,\mathbf{x}) = \phi^0(\mathbf{x})$ is expressed as

$$\begin{cases} \mathrm{i}\varepsilon\dfrac{\partial\phi_\varepsilon(t,\mathbf{x})}{\partial t} + \dfrac{\varepsilon^2}{2}\Delta\phi_\varepsilon(t,\mathbf{x}) - V\left(\dfrac{\mathbf{x}}{\varepsilon}\right)\phi_\varepsilon(t,\mathbf{x}) = 0, \quad t\in\mathbb{R}_+, \quad \mathbf{x}\in\mathbb{R}^d,\\ \phi_\varepsilon(t=0,\mathbf{x}) = \phi_\varepsilon^0(\mathbf{x}). \end{cases} \tag{2.5}$$

We define the *(asymmetric) Wigner transform* of the solution $\phi_\varepsilon(t,\mathbf{x})$ as

$$W_\varepsilon(t,\mathbf{x},\mathbf{k}) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{y}}\phi_\varepsilon(t,\mathbf{x}-\varepsilon\mathbf{y})\,\overline{\phi_\varepsilon(t,\mathbf{x})}\,\mathrm{d}\mathbf{y}, \tag{2.6}$$

then (2.5) becomes

$$\begin{aligned} &\partial_t W_\varepsilon(t,\mathbf{x},\mathbf{k}) + \mathbf{k}\cdot\nabla_{\mathbf{x}}W_\varepsilon(t,\mathbf{x},\mathbf{k}) + \frac{\mathrm{i}\varepsilon}{2}\Delta_{\mathbf{x}}W_\varepsilon(t,\mathbf{x},\mathbf{k})\\ &\quad = \frac{1}{\mathrm{i}\varepsilon}\sum_{\boldsymbol{\mu}\in\Lambda^*} \mathrm{e}^{\mathrm{i}\boldsymbol{\mu}\cdot\frac{\mathbf{x}}{\varepsilon}}\hat{V}(\boldsymbol{\mu})\left[W_\varepsilon(t,\mathbf{x},\mathbf{k}-\boldsymbol{\mu}) - W_\varepsilon(t,\mathbf{x},\mathbf{k})\right] \end{aligned} \tag{2.7}$$

with the initial condition:

$$W_\varepsilon(t=0,\mathbf{x},\mathbf{k}) = W_\varepsilon^0(\mathbf{x},\mathbf{k}) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \mathrm{e}^{-\,\mathrm{i}\mathbf{k}\cdot\mathbf{y}}\phi_\varepsilon^0(\mathbf{x}-\varepsilon\mathbf{y})\,\overline{\phi_\varepsilon^0(\mathbf{x})}\,\mathrm{d}\mathbf{y}, \tag{2.8}$$

where $\boldsymbol{\mu}\in\Lambda^*$ and

$$\hat{V}(\boldsymbol{\mu}) = \frac{1}{|\mathcal{C}|}\int_{\mathcal{C}} \mathrm{e}^{-\,\mathrm{i}\boldsymbol{\mu}\cdot\mathbf{y}}V(\mathbf{y})\,\mathrm{d}\mathbf{y}.$$

Hence, the Wigner transform provides a convenient approach for studying energy propagation in the phase space $(\mathbf{x},\mathbf{k})\in\mathbb{R}^d\times\mathbb{R}^d$. See [26, 34, 41, 25] for additional insights into the properties of the Wigner transform.

Remark 2.1. In addition to the asymmetric Wigner transform (2.6), one can alternatively use the symmetric version of the Wigner transform,

$$\tilde{W}_\varepsilon(t,\mathbf{x},\mathbf{k}) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \mathrm{e}^{-\,\mathrm{i}\mathbf{k}\cdot\mathbf{y}}\phi_\varepsilon\left(t,\mathbf{x}-\frac{\varepsilon\mathbf{y}}{2}\right)\overline{\phi_\varepsilon\left(t,\mathbf{x}+\frac{\varepsilon\mathbf{y}}{2}\right)}\,\mathrm{d}\mathbf{y},$$

which is equivalent to $W_\varepsilon(t,\mathbf{x},\mathbf{k})$ in the sense that they have the same weak limit as $\varepsilon\downarrow 0$ [3]. In the subsequent discussion, we will employ the asymmetric version as it yields a more concise result like (3.17). For further distinctions, one may refer to the discourse in [14, p. 515].

3. Semiclassical model in a periodic structure without randomness.

3.1. Derivation of effective model by asymptotic analysis. In this section, we explore the semiclassical limit of the Schrödinger equation in the absence of randomness. Without loss of generality, we specifically focus on the case where two energy bands intersect. Our derivation closely aligns with the approach outlined in [14], but extends it to arbitrary dimensions with any lattice structure. Our derivation also aligns with the method of [3], which addressed the case without band crossings.

We start by seeking a solution of (2.7) with the two-scale form

$$W_\varepsilon(t,\mathbf{x},\mathbf{k}) \mapsto W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k})|_{\mathbf{z}=\frac{\mathbf{x}}{\varepsilon}},$$

where we abuse notation to write W_ε for both the original Wigner transform and its two-scale form. We will refer to $\mathbf{z}=\frac{\mathbf{x}}{\varepsilon}$ as the fast variable. Replacing

$$\nabla_{\mathbf{x}} \mapsto \nabla_{\mathbf{x}} + \frac{1}{\varepsilon}\nabla_{\mathbf{z}}$$

in (2.7) to obtain

$$\begin{aligned}
&\partial_t W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k}) + \mathbf{k}\cdot\nabla_{\mathbf{x}}W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k}) + \frac{1}{\varepsilon}\mathbf{k}\cdot\nabla_{\mathbf{z}}W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k})\\
&\quad + \frac{\mathrm{i}\varepsilon}{2}\Delta_{\mathbf{x}}W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k}) + \mathrm{i}\nabla_{\mathbf{z}}\cdot\nabla_{\mathbf{x}}W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k}) + \frac{\mathrm{i}}{2\varepsilon}\Delta_{\mathbf{z}}W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k})\\
&= \frac{1}{\mathrm{i}\varepsilon}\sum_{\boldsymbol{\mu}\in\Lambda^*} \mathrm{e}^{\mathrm{i}\boldsymbol{\mu}\cdot\mathbf{z}}\hat{V}(\boldsymbol{\mu})\left[W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k}-\boldsymbol{\mu}) - W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k})\right],
\end{aligned} \tag{3.1}$$

we seek a solution by the formal asymptotic expansion

$$W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k}) = W_0(t,\mathbf{x},\mathbf{z},\mathbf{k}) + \varepsilon W_1(t,\mathbf{x},\mathbf{z},\mathbf{k}) + \varepsilon^2 W_2(t,\mathbf{x},\mathbf{z},\mathbf{k}) + \cdots. \tag{3.2}$$

Substituting (3.2) into (3.1) and equating terms of like order in ε, we obtain a sequence of equations.

(I) *At order* $O\left(\frac{1}{\varepsilon}\right)$, we have

$$\underbrace{\mathbf{k}\cdot\nabla_{\mathbf{z}}W_0+\frac{\mathrm{i}}{2}\Delta_{\mathbf{z}}W_0-\frac{1}{\mathrm{i}}\sum_{\boldsymbol{\mu}\in\Lambda^*}\mathrm{e}^{\mathrm{i}\boldsymbol{\mu}\cdot\mathbf{z}}\hat{V}(\boldsymbol{\mu})[W_0(t,\mathbf{x},\mathbf{z},\mathbf{k}-\boldsymbol{\mu})-W_0(t,\mathbf{x},\mathbf{z},\mathbf{k})]}_{\stackrel{\mathrm{def}}{=}\mathcal{L}[W_0](t,\mathbf{x},\mathbf{z},\mathbf{k}),}=0, \tag{3.3}$$

where we have defined the operator $\mathcal{L}$, which is skew-symmetric with respect to the inner product (3.11). For (3.3) to be satisfied, $W_0(t,\mathbf{x},\mathbf{z},\mathbf{k})$ must belong to $\mathrm{Ker}\mathcal{L}$.

To characterize $\mathrm{Ker}\mathcal{L}$, note first that any $\mathbf{k}\in\mathbb{R}^d$ can be uniquely decomposed into

$$\mathbf{k}=\mathbf{p}+\boldsymbol{\mu}\quad\text{with}\quad\mathbf{p}\in\mathcal{B}\quad\text{and}\quad\boldsymbol{\mu}\in\Lambda^*. \tag{3.4}$$

For positive integers m,n, we can define $Q_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})$ using the Bloch functions as

$$Q_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})=\frac{1}{|\mathcal{C}|}\int_{\mathcal{C}}\mathrm{e}^{\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot\mathbf{y}}\Psi_m(\mathbf{z}-\mathbf{y},\mathbf{p})\overline{\Psi_n(\mathbf{z},\mathbf{p})}\,\mathrm{d}\mathbf{y}. \tag{3.5}$$

Then $Q_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})$ is Λ-periodic in $\mathbf{z}$ and satisfies

$$\mathcal{L}[Q_{mn}](\mathbf{z},\boldsymbol{\mu},\mathbf{p})=\mathrm{i}\big(E_m(\mathbf{p})-E_n(\mathbf{p})\big)Q_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p}).$$

Clearly, we have $Q_{mm}\in\mathrm{Ker}\mathcal{L}$ for all m. For $\mathbf{p}_*$ such that $E_m(\mathbf{p}_*)=E_n(\mathbf{p}_*)$ for $m\neq n$, i.e., at band crossings (for example, Dirac points in graphene; see section 5), Q_{mn} also belongs to $\mathrm{Ker}\mathcal{L}$.

In order to describe effects arising from band crossings, following [14], we take $W_0(t,\mathbf{x},\mathbf{z},\mathbf{k})$ as

$$W_0(t,\mathbf{x},\mathbf{z},\mathbf{k})=\sum_{m,n=1}^{2}\sigma_{mn}(t,\mathbf{x},\mathbf{p})Q_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p}), \tag{3.6}$$

where $\mathbf{k}\in\mathbb{R}^d$, $\mathbf{p}\in\mathcal{B}$, and $\boldsymbol{\mu}\in\Lambda^*$ are related as described in (3.4) and σ_{mn} is called the coherence function.

Remark 3.1. A more general expansion of W_0 is

$$W_0(t,\mathbf{x},\mathbf{z},\mathbf{k})=\sum_{m,n,\alpha,\beta}\sigma_{mn}^{\alpha\beta}(t,\mathbf{x},\mathbf{p})Q_{mn}^{\alpha\beta}(\mathbf{z},\boldsymbol{\mu},\mathbf{p}), \tag{3.7}$$

where the superscripts α,β label the eigenfunctions inside the eigenspace. Since our main focus is on handling band crossings, we assume the multiplicity of each eigenvalue $E_m(\mathbf{p})$ is 1 for simplicity (this assumption is known to be true for the leading eigenvalue when the Fourier transform of the periodic potential V is negative [3]), so that no superscripts are needed in the asymptotic expansion form (3.6). Higher multiplicity will not bring essential difficulties in our following calculation.

We assume that ϕ_ε^0 in (2.5) is such that the Wigner-transformed initial condition in (2.8) can be expressed as

$$W_\varepsilon(0,\mathbf{x},\mathbf{k})=\sum_{m,n=1}^{2}\sigma_{mn}^0(\mathbf{x},\mathbf{p})Q_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})\Big|_{\mathbf{z}=\frac{\mathbf{x}}{\varepsilon}} \tag{3.8}$$

for some σ_{mn}^0. It is important to note that W_0 in the form of (3.6) does not always belong to Ker$\mathcal{L}$, so that (3.3) is not exactly satisfied. Instead, we have

$$\mathcal{L}[W_0] = \sum_{m,n=1}^{2} \sigma_{mn}(t,\mathbf{x},\mathbf{p})\mathcal{L}[Q_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})] = \sigma_{12}(t,\mathbf{x},\mathbf{p})\mathcal{L}[Q_{12}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})] + \sigma_{21}(t,\mathbf{x},\mathbf{p})\mathcal{L}[Q_{21}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})], \tag{3.9}$$

and for $\mathbf{p} \neq \mathbf{p}_*$, i.e., away from band crossings, the right-hand side is nonzero. Nevertheless, we still use the form (3.6) as it encodes the interaction between bands as we will see next.

Remark 3.2. Note that the right-hand side of (3.9) will be zero for all $\mathbf{p}$ if the bands E_m and E_n coincide everywhere, i.e., are everywhere degenerate. We ignore this case in the present work since we do not anticipate interesting new phenomena arising from this generalization. Our results will generalize, but be more complicated. For example, the coherence functions σ_{mn} appearing in (3.6) must become matrix valued.

(II) *At order* $O(1)$, we have

$$\frac{\partial W_0}{\partial t} + \mathbf{k}\cdot\nabla_{\mathbf{x}} W_0 + \mathrm{i}\nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{z}} W_0 = -\mathcal{L}[W_1] - \frac{1}{\varepsilon}\mathcal{L}[W_0]. \tag{3.10}$$

Again, $\frac{1}{\varepsilon}\mathcal{L}[W_0]$ needs to be kept because $\mathcal{L}[W_0]$ is not always zero when W_0 takes the form of (3.6).

To proceed with the derivation, we first introduce the following orthogonal relations between Q_{mn}. Let $\langle\cdot,\cdot\rangle_{\mathcal{C},\Lambda^*}$ denote integration in $\mathbf{z}$ over the fundamental cell $\mathcal{C}$ and summation over $\boldsymbol{\mu}\in\Lambda^*$, i.e.,

$$\langle f(\cdot,\cdot,\mathbf{p}), g(\cdot,\cdot,\mathbf{p})\rangle_{\mathcal{C},\Lambda^*} := \sum_{\boldsymbol{\mu}\in\Lambda^*} \frac{1}{|\mathcal{C}|}\int_{\mathcal{C}} f(\mathbf{z},\boldsymbol{\mu},\mathbf{p})\,\overline{g(\mathbf{z},\boldsymbol{\mu},\mathbf{p})}\,\mathrm{d}\mathbf{z}, \tag{3.11}$$

and $\langle\cdot,\cdot\rangle_{\mathcal{C}}$ is the integration in $\mathbf{z}$ over the fundamental cell $\mathcal{C}$,

$$\langle f(\cdot,\mathbf{p}), g(\cdot,\mathbf{p})\rangle_{\mathcal{C}} := \frac{1}{|\mathcal{C}|}\int_{\mathcal{C}} f(\mathbf{z},\mathbf{p})\,\overline{g(\mathbf{z},\mathbf{p})}\,\mathrm{d}\mathbf{z}.$$

Then, we have, for $\mathbf{p}\in\mathcal{B}$,

$$\langle Q_{mn}(\cdot,\cdot,\mathbf{p}), Q_{jl}(\cdot,\cdot,\mathbf{p})\rangle_{\mathcal{C},\Lambda^*} = \sum_{\boldsymbol{\mu}\in\Lambda^*} \frac{1}{|\mathcal{C}|}\int_{\mathcal{C}} Q_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})\,\overline{Q_{jl}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})}\,\mathrm{d}\mathbf{z} = \delta_{mj}\delta_{nl}\,; \tag{3.12}$$

and for $\mathbf{k} = \mathbf{p}+\boldsymbol{\mu}$,

$$\langle \mathbf{k}Q_{mn}(\cdot,\cdot,\mathbf{p}), Q_{jl}(\cdot,\cdot,\mathbf{p})\rangle_{\mathcal{C},\Lambda^*} = \sum_{\boldsymbol{\mu}\in\Lambda^*} \frac{1}{|\mathcal{C}|}\int_{\mathcal{C}} (\mathbf{p}+\boldsymbol{\mu}) Q_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})\,\overline{Q_{jl}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})}\,\mathrm{d}\mathbf{z} = \langle(-\mathrm{i}\nabla_z)\Psi_m(\cdot,\mathbf{p}), \Psi_j(\cdot,\mathbf{p})\rangle_{\mathcal{C}}\,\delta_{nl}\,; \tag{3.13}$$

and

$$\begin{aligned}&\langle \nabla_{\mathbf{z}}Q_{mn}(\cdot,\cdot,\mathbf{p}),\, Q_{jl}(\cdot,\cdot,\mathbf{p})\rangle_{\mathcal{C},\Lambda^*} \\ &\quad= \sum_{\boldsymbol{\mu}\in\Lambda^*} \frac{1}{|\mathcal{C}|}\int_{\mathcal{C}} \nabla_{\mathbf{z}} Q_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})\,\overline{Q_{jl}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})}\,\mathrm{d}\mathbf{z} \\ &\quad= -\langle\nabla_{\mathbf{z}}\Psi_m(\cdot,\mathbf{p}), \Psi_j(\cdot,\mathbf{p})\rangle_{\mathcal{C}}\,\delta_{nl} + \overline{\langle\nabla_{\mathbf{z}}\Psi_n(\cdot,\mathbf{p}), \Psi_l(\cdot,\mathbf{p})\rangle_{\mathcal{C}}}\,\delta_{mj}.\end{aligned} \tag{3.14}$$

We refer to [3, p. 486] for further details, and additional calculations are provided in Appendix A for completeness.

Returning to (3.10), we can obtain the equation for W_0 by imposing a solvability condition on the equation for W_1. Specifically, taking the inner product on both sides of (3.10) with Q_{jl} $(j,l\in\{1,2\})$ in $\mathbf{z}$ and $\boldsymbol{\mu}$, we have

$$\sum_{m,n=1}^{2}\Big[\langle\partial_t\sigma_{mn}Q_{mn},Q_{jl}\rangle_{\mathcal{C},\Lambda^*}+\langle\mathbf{k}\cdot\nabla_{\mathbf{x}}\sigma_{mn}Q_{mn},Q_{jl}\rangle_{\mathcal{C},\Lambda^*}+\langle \mathrm{i}\nabla_{\mathbf{z}}\cdot\nabla_{\mathbf{x}}\sigma_{mn}Q_{mn},Q_{jl}\rangle_{\mathcal{C},\Lambda^*}\Big]$$
$$=\langle\mathcal{L}[W_1],Q_{jl}\rangle_{\mathcal{C},\Lambda^*}-\frac{1}{\varepsilon}\sum_{m,n=1}^{2}\langle\sigma_{mn}\mathcal{L}[Q_{mn}],Q_{jl}\rangle_{\mathcal{C},\Lambda^*},$$

which is further simplified as follows:

$$\begin{aligned}&\sum_{m,n=1}^{2}\Big[\partial_t\sigma_{mn}\langle Q_{mn},Q_{jl}\rangle_{\mathcal{C},\Lambda^*}+\nabla_{\mathbf{x}}\sigma_{mn}\cdot\langle\mathbf{k}Q_{mn},Q_{jl}\rangle_{\mathcal{C},\Lambda^*}+\mathrm{i}\nabla_{\mathbf{x}}\sigma_{mn}\cdot\langle\nabla_{\mathbf{z}}Q_{mn},Q_{jl}\rangle_{\mathcal{C},\Lambda^*}\Big]\\&=-\langle W_1,\mathcal{L}[Q_{jl}]\rangle_{\mathcal{C},\Lambda^*}-\sum_{m,n=1}^{2}\sigma_{mn}\frac{\mathrm{i}}{\varepsilon}[E_m(\mathbf{p})-E_n(\mathbf{p})]\langle Q_{mn},Q_{jl}\rangle_{\mathcal{C},\Lambda^*}\\&=\mathrm{i}[E_l(\mathbf{p})-E_j(\mathbf{p})]\langle W_1,Q_{jl}\rangle_{\mathcal{C},\Lambda^*}-\sum_{m,n=1}^{2}\sigma_{mn}\frac{\mathrm{i}}{\varepsilon}[E_m(\mathbf{p})-E_n(\mathbf{p})]\langle Q_{mn},Q_{jl}\rangle_{\mathcal{C},\Lambda^*}.\end{aligned}\tag{3.15}$$

Note that the term $\mathrm{i}[E_l(\mathbf{p})-E_j(\mathbf{p})]\langle W_1,Q_{jl}\rangle_{\mathcal{C},\Lambda^*}$ can be considered negligible. The rationale is as follows: when $\mathbf{p}=\mathbf{p}_*$, where $\mathbf{p}_*$ is the band crossings point, i.e., $E_1(\mathbf{p}_*)=E_2(\mathbf{p}_*)$, this term becomes zero. In a small neighborhood of $\mathbf{p}_*$, where $\mathbf{p}$ is close to $\mathbf{p}_*$, the quantity $|E_1(\mathbf{p})-E_2(\mathbf{p})|$ is much smaller than 1. Furthermore, when $\mathbf{p}$ is far away from $\mathbf{p}_*$ and the two bands are well-separated, one should follow the derivation in [3] for well-separated energy bands, where this term no longer appears. For these reasons, we drop this term in what follows.

By substituting the orthogonality conditions (3.12), (3.13), and (3.14), we can simplify (3.15) into

$$\partial_t\sigma_{jl}+\sum_{n=1}^{2}\nabla_{\mathbf{x}}\sigma_{jn}\cdot\langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_l,\Psi_n\rangle_{\mathcal{C}}=\frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p})-E_j(\mathbf{p})]\sigma_{jl},\quad j,l\in\{1,2\},\tag{3.16}$$

which must be solved subject to the initial condition

$$\sigma_{jl}(0,\mathbf{x},\mathbf{p})=\sigma_{jl}^0(\mathbf{x},\mathbf{p}),\quad j,l\in\{1,2\},$$

where σ_{jl}^0 are as in (3.8). We refer to the term on the right-hand side of (3.16) as a relaxation-type term because of its similarity to terms appearing in the models of kinetic theory and conservation law; see [10, 29]. The system (3.16) can be written in the following matrix form,

$$\begin{aligned}&\partial_t\begin{pmatrix}\sigma_{11}&\sigma_{12}\\\sigma_{21}&\sigma_{22}\end{pmatrix}+\nabla_{\mathbf{x}}\begin{pmatrix}\sigma_{11}&\sigma_{12}\\\sigma_{21}&\sigma_{22}\end{pmatrix}\cdot\begin{pmatrix}\langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_1,\Psi_1\rangle_{\mathcal{C}}&\langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_2,\Psi_1\rangle_{\mathcal{C}}\\\langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_1,\Psi_2\rangle_{\mathcal{C}}&\langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_2,\Psi_2\rangle_{\mathcal{C}}\end{pmatrix}\\&=\frac{\mathrm{i}}{\varepsilon}\begin{pmatrix}0&[E_2(\mathbf{p})-E_1(\mathbf{p})]\sigma_{12}\\{[E_1(\mathbf{p})-E_2(\mathbf{p})]\sigma_{21}}&0\end{pmatrix},\end{aligned}\tag{3.17}$$

where we have introduced the convenient shorthand notation

$$\nabla_{\mathbf{x}} \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \cdot \begin{pmatrix} \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_1, \Psi_1\rangle_{\mathcal{C}} & \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_2, \Psi_1\rangle_{\mathcal{C}} \\ \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_1, \Psi_2\rangle_{\mathcal{C}} & \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_2, \Psi_2\rangle_{\mathcal{C}} \end{pmatrix}$$
$$:= \sum_{i=1}^{d} \begin{pmatrix} \partial_{x_i}\sigma_{11} & \partial_{x_i}\sigma_{12} \\ \partial_{x_i}\sigma_{21} & \partial_{x_i}\sigma_{22} \end{pmatrix} \begin{pmatrix} \langle(-\mathrm{i}\partial_{z_i})\Psi_1, \Psi_1\rangle_{\mathcal{C}} & \langle(-\mathrm{i}\partial_{z_i})\Psi_2, \Psi_1\rangle_{\mathcal{C}} \\ \langle(-\mathrm{i}\partial_{z_i})\Psi_1, \Psi_2\rangle_{\mathcal{C}} & \langle(-\mathrm{i}\partial_{z_i})\Psi_2, \Psi_2\rangle_{\mathcal{C}} \end{pmatrix}.$$

We can write (3.17) more concisely by introducing

$$\sigma := \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix}, \quad D := \begin{pmatrix} \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_1, \Psi_1\rangle_{\mathcal{C}} & \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_2, \Psi_1\rangle_{\mathcal{C}} \\ \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_1, \Psi_2\rangle_{\mathcal{C}} & \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_2, \Psi_2\rangle_{\mathcal{C}} \end{pmatrix},$$

$$E := \frac{\mathrm{i}}{\varepsilon} \begin{pmatrix} 0 & [E_2(\mathbf{p}) - E_1(\mathbf{p})]\sigma_{12} \\ [E_1(\mathbf{p}) - E_2(\mathbf{p})]\sigma_{21} & 0 \end{pmatrix}, \quad \sigma^0 := \begin{pmatrix} \sigma_{11}^0 & \sigma_{12}^0 \\ \sigma_{21}^0 & \sigma_{22}^0 \end{pmatrix}.$$

The system (3.17) can then be presented as

$$\partial_t \sigma + \nabla_{\mathbf{x}}\sigma \cdot D = E, \quad \sigma(0) = \sigma^0.$$

Remark 3.3. Noting that $\overline{D^T} = D$, taking the complex conjugate and transpose of (3.17) we see that $\overline{\sigma^T}$ satisfies an equivalent system to (3.17), where D acts by matrix multiplication from the left:

$$\partial_t \overline{\sigma^T} + \overline{D^T} \cdot \nabla_x \overline{\sigma^T} = \partial_t \overline{\sigma^T} + D \cdot \nabla_x \overline{\sigma^T} = \overline{E^T}.$$

3.2. Alternative formulation and domain decomposition of the derived model. The preceding calculation shows that making the ansatz (3.6) produces terms proportional to $\frac{1}{\varepsilon}$ in (3.17). This idea for dealing with systems with crossings goes back to [14] but still demands further explanation and justification since these terms seem to invalidate the asymptotic expansion. We now show how the system (3.17) reduces to the Liouville equation for $\mathbf{p}$ when the bands are well-separated, while still capturing the diabatic (band crossing) effect for $\mathbf{p}$ when the bands are close or touching.

We start by introducing

$$\widetilde{\sigma}_{jl}(t, \mathbf{x}, \mathbf{p}) := \mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}[E_j(\mathbf{p}) - E_l(\mathbf{p})]t} \sigma_{jl}(t, \mathbf{x}, \mathbf{p}), \quad j, l \in \{1, 2\}, \tag{3.18}$$

and then rewrite the system (3.17) as a system for $\widetilde{\sigma}_{jl}$ as

$$\partial_t \widetilde{\sigma}_{jl}(t, \mathbf{x}, \mathbf{p}) + \sum_{n=1}^{2} \nabla_{\mathbf{x}} \widetilde{\sigma}_{jn}(t, \mathbf{x}, \mathbf{p}) \cdot \mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p}) - E_n(\mathbf{p})]t} \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_l, \Psi_n\rangle_{\mathcal{C}} = 0, \tag{3.19}$$

or in matrix form (clearly, $\widetilde{\sigma}_{jl} = \sigma_{jl}$ for $j = l$),

(3.20)
$$\mathbf{0} = \partial_t \begin{pmatrix} \sigma_{11} & \widetilde{\sigma}_{12} \\ \widetilde{\sigma}_{21} & \sigma_{22} \end{pmatrix} + \nabla_{\mathbf{x}} \begin{pmatrix} \sigma_{11} & \widetilde{\sigma}_{12} \\ \widetilde{\sigma}_{21} & \sigma_{22} \end{pmatrix}$$
$$\cdot \begin{pmatrix} \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_1, \Psi_1\rangle_{\mathcal{C}} & \mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}[E_2(\mathbf{p}) - E_1(\mathbf{p})]t} \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_2, \Psi_1\rangle_{\mathcal{C}} \\ \mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}[E_1(\mathbf{p}) - E_2(\mathbf{p})]t} \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_1, \Psi_2\rangle_{\mathcal{C}} & \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_2, \Psi_2\rangle_{\mathcal{C}} \end{pmatrix}.$$

We can now extract the limiting behavior of solutions of (3.19), and hence of (3.17), in the limit $\varepsilon \downarrow 0$ for different values of $\mathbf{p}$. For simplicity, we assume at this point that

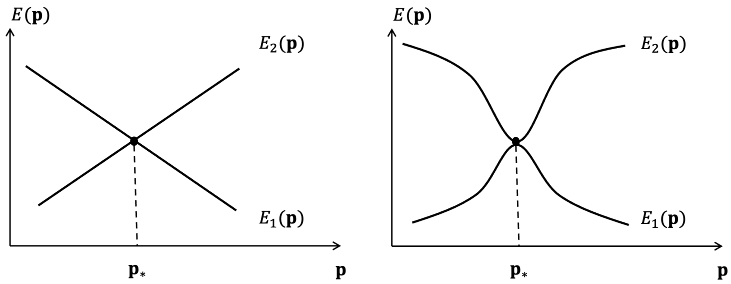

FIG. 1. *Left: A conical* ($r = 1$) *energy band crossing. Right: A quadratic* ($r = 2$) *energy band crossing.*

the bands E_1, E_2 have finitely many separated crossing points $\mathbf{p}_*$. The case where eigenvalues cross along a curve can be dealt with similarly. We then assume that in a neighborhood of each $\mathbf{p}_*$ the crossing has the following structure,

$$E_1(\mathbf{p}) = -\lambda_\sharp|\mathbf{p} - \mathbf{p}_*|^r + o(|\mathbf{p} - \mathbf{p}_*|^r), \quad E_2(\mathbf{p}) = \lambda_\sharp|\mathbf{p} - \mathbf{p}_*|^r + o(|\mathbf{p} - \mathbf{p}_*|^r), \quad \mathbf{p} \to \mathbf{p}_* \tag{3.21}$$

for some positive constants $\lambda_\sharp$ and positive integers $r > 0$. This assumption allows for both conical ($r = 1$) and quadratic ($r = 2$) crossings; see Figure 1. The case $r = 1$ is the situation encountered in graphene (see (5.1)), while $r = 2$ occurs in untwisted and twisted bilayer graphene [37, 7].

We then have the following dichotomy about the domain decomposition, depending on the nature of the crossing.

- When $|\mathbf{p} - \mathbf{p}_*| \gg \varepsilon^{1/r}$ as $\varepsilon \downarrow 0$, the functions $\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p}) - E_n(\mathbf{p})]}$ are highly oscillatory with mean zero as $\varepsilon \downarrow 0$ for $l \neq n$. By standard arguments (see, e.g., [1]), the solution of (3.19) converges weakly to the solution of the following system,

$$\partial_t \widetilde{\sigma}_{jl}(t, \mathbf{x}, \mathbf{p}) + \nabla_{\mathbf{x}} \widetilde{\sigma}_{jl}(t, \mathbf{x}, \mathbf{p}) \cdot \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_l, \Psi_l\rangle_{\mathcal{C}} = 0, \quad j, l \in \{1, 2\}, \tag{3.22}$$

  which is obtained by replacing the relaxation term $\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p}) - E_n(\mathbf{p})]}$ in (3.19) with δ_{ln}. When these equations are expressed in terms of the eigenvalue band functions we recover the familiar form of the Liouville equation

$$\partial_t \widetilde{\sigma}_{jl} + \nabla_{\mathbf{p}} E_l(\mathbf{p}) \cdot \nabla_{\mathbf{x}} \widetilde{\sigma}_{jl} = 0, \quad j, l \in \{1, 2\}. \tag{3.23}$$

  In particular, we recover the result of [3], since when $\widetilde{\sigma}_{12}$ and $\widetilde{\sigma}_{21}$ are initially zero, they remain zero for each positive t in the limit $\varepsilon \downarrow 0$, while σ_{11} and σ_{22} evolve according to the same Liouville equations as derived in [3, eq. (2.24)].
- When $|\mathbf{p} - \mathbf{p}_*| = O(\varepsilon^{1/r})$ as $\varepsilon \downarrow 0$, the functions $\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p}) - E_n(\mathbf{p})]}$ are no longer highly oscillatory and cannot be replaced by δ_{ln}. In particular, in this regime the coupling between the diagonal entries σ_{11} and σ_{22} to the off-diagonal entries $\widetilde{\sigma}_{12}$ and $\widetilde{\sigma}_{21}$ is no longer $o(1)$ as $\varepsilon \downarrow 0$, reflecting the fact that in this regime interband coupling effects cannot be ignored. Note also that in this regime the terms $\frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p}) - E_j(\mathbf{p})]$ in (3.17) no longer blow up as $\varepsilon \downarrow 0$.

We thus have that, even though the system (3.17) involves terms proportional to $\frac{1}{\varepsilon}$, its solutions make sense in every case and indeed reduce to previously known results as expected. We remark further that the terms proportional to $\frac{1}{\varepsilon}$ in the expansion could be removed from the beginning of the calculation by setting, instead of as in (3.6),

$$W_0(t,\mathbf{x},\mathbf{z},\mathbf{k}) = \sum_{m,n=1}^{2} \mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}[E_m(\mathbf{p})-E_n(\mathbf{p})]t} \sigma_{mn}(t,\mathbf{x},\mathbf{p}) Q_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p}). \tag{3.24}$$

Equating terms of order $O(1)$ in the expansion would then give (3.19) directly. Since the models obtained are ultimately equivalent, and the calculations become somewhat more complicated in the random case if we make the ansatz (3.24), we prefer to make the ansatz (3.6).

4. Semiclassical model in a periodic structure with randomness. We now consider a weak random perturbation of the problem (2.5) as follows:

$$\begin{cases} \mathrm{i}\varepsilon \dfrac{\partial \phi_\varepsilon}{\partial t} + \dfrac{\varepsilon^2}{2}\Delta_{\mathbf{x}}\phi_\varepsilon - V\left(\dfrac{\mathbf{x}}{\varepsilon}\right)\phi_\varepsilon - \sqrt{\varepsilon}N\left(\dfrac{\mathbf{x}}{\varepsilon}\right)\phi_\varepsilon = 0, \\ \phi_\varepsilon(t=0,\mathbf{x}) = \phi_\varepsilon^0(\mathbf{x}). \end{cases} \tag{4.1}$$

Here N is a stationary, real-valued mean zero, spatially homogeneous random function on the probability space $(\Omega,\mathcal{F},\mathbb{P})$ with covariance given by

$$\mathbb{E}[N(\mathbf{y})N(\mathbf{y}+\mathbf{x})] = R(\mathbf{x}), \quad \mathbb{E}[\hat{N}(\mathbf{p})\hat{N}(\mathbf{q})] = (2\pi)^d \hat{R}(\mathbf{q})\,\delta(\mathbf{p}+\mathbf{q}), \tag{4.2}$$

where $\hat{N}(\mathbf{q})$ is the Fourier transform of $N(\mathbf{y})$:

$$\hat{N}(\mathbf{q}) = \int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{y}} N(\mathbf{y})\,\mathrm{d}\mathbf{y}.$$

By the scaling of N in (4.1), we are considering a random inhomogeneity with correlation length comparable to the wavelength ε and a small variance.

Upon applying the Wigner transform to both sides of (4.1), we obtain

$$\begin{aligned} &\partial_t W_\varepsilon + \mathbf{k}\cdot\nabla_{\mathbf{x}}W_\varepsilon + \frac{\mathrm{i}\varepsilon}{2}\Delta_{\mathbf{x}}W_\varepsilon \\ &\quad = \frac{1}{\mathrm{i}\varepsilon}\sum_{\boldsymbol{\mu}\in\Lambda^*} \mathrm{e}^{\mathrm{i}\boldsymbol{\mu}\cdot\mathbf{z}}\hat{V}(\boldsymbol{\mu})\,[W_\varepsilon(t,\mathbf{x},\mathbf{k}-\boldsymbol{\mu}) - W_\varepsilon(t,\mathbf{x},\mathbf{k})] \\ &\qquad + \frac{1}{\mathrm{i}\sqrt{\varepsilon}}\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\hat{N}(\mathbf{q})[W_\varepsilon(t,\mathbf{x},\mathbf{k}-\mathbf{q}) - W_\varepsilon(t,\mathbf{x},\mathbf{k})]\,\mathrm{d}\mathbf{q}, \end{aligned} \tag{4.3}$$

where $\boldsymbol{\mu}\in\Lambda^*$, $\mathbf{p}\in\mathcal{B}$, $\mathbf{q}\in\mathbb{R}^d$. Similarly to the previous section, we introduce the fast variable $\mathbf{z} = \frac{\mathbf{x}}{\varepsilon}$ in $W_\varepsilon(t,\mathbf{x},\mathbf{k})$ and express the solution as $W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k})$. Then, (4.3) can be rewritten as follows:

$$\begin{aligned} &\partial_t W_\varepsilon + \mathbf{k}\cdot\nabla_{\mathbf{x}}W_\varepsilon + \frac{1}{\varepsilon}\mathbf{k}\cdot\nabla_{\mathbf{z}}W_\varepsilon + \frac{\mathrm{i}\varepsilon}{2}\Delta_{\mathbf{x}}W_\varepsilon + \mathrm{i}\nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{z}}W_\varepsilon + \frac{\mathrm{i}}{2\varepsilon}\Delta_{\mathbf{z}}W_\varepsilon \\ &\quad = \frac{1}{\mathrm{i}\varepsilon}\sum_{\boldsymbol{\mu}\in\Lambda^*} \mathrm{e}^{\mathrm{i}\boldsymbol{\mu}\cdot\mathbf{z}}\hat{V}(\boldsymbol{\mu})\,[W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k}-\boldsymbol{\mu}) - W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k})] \\ &\qquad + \frac{1}{\mathrm{i}\sqrt{\varepsilon}}\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \hat{N}(\mathbf{q})[W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k}-\mathbf{q}) - W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k})]\,\mathrm{d}\mathbf{q}. \end{aligned} \tag{4.4}$$

Now we conduct the asymptotic analysis by substituting the following expansion into (4.4):

$$W_\varepsilon(t,\mathbf{x},\mathbf{z},\mathbf{k}) = W_0(t,\mathbf{x},\mathbf{z},\mathbf{k}) + \sqrt{\varepsilon}W_1(t,\mathbf{x},\mathbf{z},\mathbf{k}) + \varepsilon W_2(t,\mathbf{x},\mathbf{z},\mathbf{k}) + \cdots.$$

Equating terms with like orders, we obtain the following equations.

(I) *At* $O(\frac{1}{\varepsilon})$, the equation reads

$$\mathcal{L}[W_0](t,\mathbf{x},\mathbf{z},\mathbf{k}) = 0.$$

Following the same reasoning as in the deterministic case, W_0 assumes the identical form to the expression in (3.6). Notably, in (3.6), $\sigma_{mn}(t,\mathbf{x},\mathbf{p})$ is initially defined for $\mathbf{p} \in \mathcal{B}$. Nevertheless, it is viable to extend this definition periodically, ensuring Λ^*-periodicity in $\mathbf{p}$. This extension is admissible due to the Λ^*-periodicity of Q_{mn} defined in (3.5) with respect to $\mathbf{p}$.

(II) *At* $O(\frac{1}{\sqrt{\varepsilon}})$, we have

$$\mathcal{L}[W_1](t,\mathbf{x},\mathbf{z},\mathbf{k}) = \frac{1}{\mathrm{i}}\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\hat{N}(\mathbf{q})[W_0(t,\mathbf{x},\mathbf{z},\mathbf{k}-\mathbf{q}) - W_0(t,\mathbf{x},\mathbf{z},\mathbf{k})]\,\mathrm{d}\mathbf{q} \tag{4.5}$$

from which we aim to derive an explicit formula for W_1. Since W_1 need not be periodic in $\mathbf{z}$, it may not be expanded in Q_{mn}. Instead, we define

$$P_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p},\mathbf{q}) = \frac{1}{|\mathcal{C}|}\int_{\mathcal{C}} \mathrm{e}^{\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot\mathbf{y}}\Psi_m(\mathbf{z}-\mathbf{y},\mathbf{p})\,\overline{\Psi_n(\mathbf{z},\mathbf{p}+\mathbf{q})}\,\mathrm{d}\mathbf{y}$$

for $\mathbf{z} \in \mathbb{R}^d$ and $\mathbf{p},\mathbf{q} \in \mathcal{B}$. Here Ψ_m and Ψ_n are the Bloch states defined in (2.1). Then, P_{mn} are Λ-quasi-periodic in $\mathbf{z}$, i.e.,

$$P_{mn}(\mathbf{z}+\boldsymbol{\nu},\boldsymbol{\mu},\mathbf{p},\mathbf{q}) = P_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p},\mathbf{q})\,\mathrm{e}^{-\,\mathrm{i}\boldsymbol{\nu}\cdot\mathbf{q}}.$$

Utilizing (2.4) and (A.3), one can verify that P_{mn} adheres to the following orthogonal property:

$$\sum_{\boldsymbol{\mu}\in\Lambda^*}\frac{1}{|\mathcal{B}|}\int_{\mathbb{R}^d} P_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p},\mathbf{q})\,\overline{P_{jl}(\mathbf{z},\boldsymbol{\mu},\mathbf{p},\mathbf{q}_0)}\,\mathrm{d}\mathbf{z} = \delta_{mj}\delta_{nl}\delta_{\mathrm{per}}(\mathbf{q}-\mathbf{q}_0). \tag{4.6}$$

Additionally,

$$\mathcal{L}[P_{mn}] = \mathrm{i}(E_m(\mathbf{p}) - E_n(\mathbf{p}+\mathbf{q}))P_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p},\mathbf{q}).$$

We seek $W_1(t,\mathbf{x},\mathbf{z},\mathbf{p}+\boldsymbol{\mu})$ in the following form,

$$W_1(t,\mathbf{x},\mathbf{z},\mathbf{p}+\boldsymbol{\mu}) = \sum_{m,n=1}^{2}\frac{1}{|\mathcal{B}|}\int_{\mathcal{B}} \eta_{mn}(t,\mathbf{x},\mathbf{p},\mathbf{q})\,P_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p},\mathbf{q})\,\mathrm{d}\mathbf{q} \tag{4.7}$$

for $\mathbf{z} \in \mathbb{R}^d$, $\mathbf{p} \in \mathcal{B}$, and $\boldsymbol{\mu} \in \Lambda^*$, where the η_{mn} are to be determined.

More specifically, by substituting W_1 from (4.7) back into (4.5) and multiplying both sides of (4.5) by $\overline{P_{jl}(\mathbf{z},\boldsymbol{\mu},\mathbf{p},\mathbf{q}_0)}$, integrating over $\mathbf{z} \in \mathbb{R}^d$, and summing over $\boldsymbol{\mu} \in \Lambda^*$, we discover that the left-hand side (L.H.S.) of (4.5) transforms into

$$\begin{aligned} \text{L.H.S} &= \langle \mathcal{L}[W_1](t,\mathbf{x},\mathbf{z},\mathbf{k}), P_{jl}(\mathbf{z},\boldsymbol{\mu},\mathbf{p},\mathbf{q}_0)\rangle_{\mathcal{C},\Lambda^*} \\ &= \sum_{\boldsymbol{\mu}\in\Lambda^*}\int_{\mathbb{R}^d}\frac{1}{|\mathcal{B}|}\sum_{m,n=1}^{2}\int_{\mathcal{B}} \eta_{mn}\,\mathrm{i}[E_m(\mathbf{p}) - E_n(\mathbf{p}+\mathbf{q})]P_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p},\mathbf{q}) \\ &\quad\times \overline{P_{jl}(\mathbf{z},\boldsymbol{\mu},\mathbf{p},\mathbf{q}_0)}\,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{z} \\ &= \sum_{m,n=1}^{2}\int_{\mathcal{B}} \eta_{mn}\,\mathrm{i}[E_m(\mathbf{p}) - E_n(\mathbf{p}+\mathbf{q})]\delta_{mj}\delta_{nl}\delta_{\mathrm{per}}(\mathbf{q}-\mathbf{q}_0)\,\mathrm{d}\mathbf{q} \\ &= \mathrm{i}\eta_{jl}[E_j(\mathbf{p}) - E_l(\mathbf{p}+\mathbf{q}_0)], \quad \mathbf{p},\ \mathbf{q}_0 \in \mathcal{B}. \end{aligned} \tag{4.8}$$

The right-hand side (R.H.S.) of (4.5) is

$$\text{R.H.S} = \frac{1}{\mathrm{i}}\frac{1}{(2\pi)^d}\sum_{\boldsymbol{\mu}\in\Lambda^*}\frac{1}{|\mathcal{B}|}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\hat{N}(\mathbf{q})[W_0(t,\mathbf{x},\mathbf{z},\mathbf{p}+\boldsymbol{\mu}-\mathbf{q}) - W_0(t,\mathbf{x},\mathbf{z},\mathbf{p}+\boldsymbol{\mu})]\overline{P_{jl}(\mathbf{z},\boldsymbol{\mu},\mathbf{p},\mathbf{q}_0)}\,\mathrm{d}\mathbf{z}\,\mathrm{d}\mathbf{q}. \tag{4.9}$$

Comparing (4.8) with (4.9), we have that

$$\eta_{jl}(t,\mathbf{x},\mathbf{p},\mathbf{q}_0) = \frac{1}{(2\pi)^d}\sum_{\boldsymbol{\mu}\in\Lambda^*}\frac{1}{|\mathcal{B}|}\times\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\hat{N}(\mathbf{q}) \times\frac{[W_0(t,\mathbf{x},\mathbf{z},\mathbf{p}+\boldsymbol{\mu}-\mathbf{q}) - W_0(t,\mathbf{x},\mathbf{z},\mathbf{p}+\boldsymbol{\mu})]}{E_l(\mathbf{p}+\mathbf{q}_0)-E_j(\mathbf{p})+\mathrm{i}\theta}\overline{P_{jl}(\mathbf{z},\boldsymbol{\mu},\mathbf{p},\mathbf{q}_0)}\,\mathrm{d}\mathbf{z}\,\mathrm{d}\mathbf{q}, \tag{4.10}$$

where $\theta > 0$ is introduced as a regularizing parameter and will be set to zero eventually. By substituting the expression for W_0 from (3.6) into (4.10) and conducting a lengthy derivation, we arrive at, for $j,l\in\{1,2\}$,

$$\begin{aligned}\eta_{jl}(t,\mathbf{x},\mathbf{p},\mathbf{q}_0) &= \frac{1}{(2\pi)^d}\sum_{\boldsymbol{\mu}\in\Lambda^*}\frac{\hat{N}(-\boldsymbol{\mu}-\mathbf{q}_0)\sum_{m,n=1}^{2}\sigma_{mn}(\mathbf{p}+\mathbf{q}_0)\delta_{nl}}{E_l(\mathbf{p}+\mathbf{q}_0)-E_j(\mathbf{p})+\mathrm{i}\theta}A_{mj}(\mathbf{p}+\mathbf{q}_0+\boldsymbol{\mu},\mathbf{p})\\ &\quad-\frac{1}{(2\pi)^d}\frac{1}{|\mathcal{B}|}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\frac{\hat{N}(\mathbf{q})\sum_{m,n=1}^{2}\sigma_{mn}(\mathbf{p})\delta_{mj}}{E_l(\mathbf{p}+\mathbf{q}_0)-E_j(\mathbf{p})+\mathrm{i}\theta}\Psi_l(\mathbf{z},\mathbf{p}+\mathbf{q}_0)\\ &\quad\times\overline{\Psi_n(\mathbf{z},\mathbf{p})}\,\mathrm{d}\mathbf{z}\,\mathrm{d}\mathbf{q} =: (I)+(II),\end{aligned} \tag{4.11}$$

where $A_{mj}(\mathbf{q},\mathbf{p})$ is defined by

$$A_{mj}(\mathbf{q},\mathbf{p}) = \frac{1}{|\mathcal{C}|}\int_{\mathcal{C}}\mathrm{e}^{-\mathrm{i}(\mathbf{q}-\mathbf{p})\cdot\mathbf{y}}\Psi_m(\mathbf{y},\mathbf{q})\,\overline{\Psi_j(\mathbf{y},\mathbf{p})}\,\mathrm{d}\mathbf{y}.$$

The detailed derivation from (4.10) to (4.11) can be found in Appendix B.

(III) *At* $O(1)$, the equation reads

$$\begin{aligned}&\frac{\partial W_0}{\partial t}+\mathbf{k}\cdot\nabla_{\mathbf{x}}W_0+\mathrm{i}\nabla_{\mathbf{z}}\cdot\nabla_{\mathbf{x}}W_0+\mathcal{L}[W_2]\\ &\quad=\frac{1}{\mathrm{i}}\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\hat{N}(\mathbf{q})[W_1(t,\mathbf{x},\mathbf{z},\mathbf{k}-\mathbf{q})-W_1(t,\mathbf{x},\mathbf{z},\mathbf{k})]\,\mathrm{d}\mathbf{q}-\frac{1}{\varepsilon}\mathcal{L}[W_0].\end{aligned} \tag{4.12}$$

To derive the system satisfied by σ_{jl} with $j,l\in\{1,2\}$, it is necessary to multiply both sides of (4.12) by $\overline{Q_{jl}(\mathbf{z},\boldsymbol{\mu}_1,\mathbf{p})}$, integrate over $\mathbf{z}\in\mathbb{R}^d$, and sum over $\boldsymbol{\mu}_1\in\Lambda^*$ (Here the subscript of $\boldsymbol{\mu}$ is just added to distinguish different $\boldsymbol{\mu}$'s that appear later on). The resulting equation is as follows.

On the L.H.S., following a similar derivation as in the deterministic case, we have

$$\text{L.H.S} = \partial_t\sigma_{jl}+\sum_{n=1}^{2}\nabla_{\mathbf{x}}\sigma_{jn}\cdot\langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_l,\Psi_n\rangle_{\mathcal{C}}+\langle\mathcal{L}[W_2],Q_{jl}\rangle_{\mathcal{C},\Lambda^*}. \tag{4.13}$$

As elucidated similarly in (3.15), in what follows we will neglect the last term above.

On the R.H.S. we see that

$$\begin{aligned}
\text{R.H.S} &= \frac{1}{\mathrm{i}} \frac{1}{(2\pi)^d} \frac{1}{|\mathcal{C}|} \sum_{\boldsymbol{\mu}_1 \in \Lambda^*} \int_{\mathcal{C}} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}} \hat{N}(\mathbf{q}) W_1(t,\mathbf{x},\mathbf{z},\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q}) \overline{Q_{jl}(\mathbf{z},\boldsymbol{\mu}_1,\mathbf{p})} \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{z} \\
&\quad - \frac{1}{\mathrm{i}} \frac{1}{(2\pi)^d} \frac{1}{|\mathcal{C}|} \sum_{\boldsymbol{\mu}_1 \in \Lambda^*} \int_{\mathcal{C}} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}} \hat{N}(\mathbf{q}) W_1(t,\mathbf{x},\mathbf{z},\mathbf{p}+\boldsymbol{\mu}_1) \overline{Q_{jl}(\mathbf{z},\boldsymbol{\mu}_1,\mathbf{p})} \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{z} \\
&\quad - \frac{1}{\varepsilon} \langle \mathcal{L}[W_0], Q_{jl} \rangle_{\mathcal{C},\Lambda^*} \\
&= I_1 + I_2 + \frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p}) - E_j(\mathbf{p})]\sigma_{jl}\,.
\end{aligned}$$

For I_1, inserting the formula (4.7) for W_1, we have

$$\begin{aligned}
I_1 &= \frac{1}{\mathrm{i}} \frac{1}{(2\pi)^d} \frac{1}{|\mathcal{C}|} \sum_{\boldsymbol{\mu}_1 \in \Lambda^*} \int_{\mathcal{C}} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}} \hat{N}(\mathbf{q}) \sum_{m,n=1}^{2} \frac{1}{|\mathcal{B}|} \int_{\mathcal{B}} \eta_{mn}(t,\mathbf{x},\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q},\mathbf{q}_0) \\
&\quad \times P_{mn}(\mathbf{z},\boldsymbol{\mu}_1,\mathbf{p}-\mathbf{q},\mathbf{q}_0) \overline{Q_{jl}(\mathbf{z},\boldsymbol{\mu}_1,\mathbf{p})} \,\mathrm{d}\mathbf{q}_0\,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{z},
\end{aligned}$$

which, upon substituting (4.11) of η_{mn}, becomes

$$\begin{aligned}
I_1 &= \frac{1}{\mathrm{i}} \frac{1}{(2\pi)^d} \frac{1}{|\mathcal{C}|} \sum_{\boldsymbol{\mu}_1 \in \Lambda^*} \int_{\mathcal{C}} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}} \hat{N}(\mathbf{q}) \sum_{m,n=1}^{2} \frac{1}{|\mathcal{B}|} \\
&\quad \times \int_{\mathcal{B}} \frac{1}{(2\pi)^d} \sum_{\boldsymbol{\mu}_2 \in \Lambda^*} \frac{\hat{N}(-\boldsymbol{\mu}_2-\mathbf{q}_0) \sum_{m',n'=1}^{2} \sigma_{m'n'}((\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})+\mathbf{q}_0)\delta_{n'n}}{E_n((\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})+\mathbf{q}_0) - E_m((\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})) + \mathrm{i}\theta} \\
&\quad \times A_{m'm}((\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})+\mathbf{q}_0+\boldsymbol{\mu}_2,(\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})) \\
&\quad \times P_{mn}(\mathbf{z},\boldsymbol{\mu}_1,\mathbf{p}-\mathbf{q},\mathbf{q}_0) \overline{Q_{jl}(\mathbf{z},\boldsymbol{\mu}_1,\mathbf{p})} \,\mathrm{d}\mathbf{q}_0\,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{z} \\
&\quad - \frac{1}{\mathrm{i}} \frac{1}{(2\pi)^d} \frac{1}{|\mathcal{B}|} \frac{1}{|\mathcal{C}|} \sum_{\boldsymbol{\mu}_1 \in \Lambda^*} \int_{\mathcal{C}} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}} \hat{N}(\mathbf{q}) \sum_{m,n=1}^{2} \frac{1}{|\mathcal{B}|} \\
&\quad \times \int_{\mathcal{B}} \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\mathbf{q}_1\cdot\mathbf{z}_1} \frac{\hat{N}(\mathbf{q}_1) \sum_{m',n'=1}^{2} \sigma_{m'n'}((\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q}))\delta_{mm'}}{E_n((\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})+\mathbf{q}_0) - E_m((\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})) + \mathrm{i}\theta} \\
&\quad \times \Psi_n(\mathbf{z}_1,(\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})+\mathbf{q}_0) \overline{\Psi_{n'}(\mathbf{z}_1,(\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q}))} \,\mathrm{d}\mathbf{z}_1\,\mathrm{d}\mathbf{q}_1 \\
&\quad \times P_{mn}(\mathbf{z},\boldsymbol{\mu}_1,\mathbf{p}-\mathbf{q},\mathbf{q}_0) \overline{Q_{jl}(\mathbf{z},\boldsymbol{\mu}_1,\mathbf{p})} \,\mathrm{d}\mathbf{q}_0\,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{z} \\
&=: I_{11} - I_{12}.
\end{aligned}$$

For the term I_{11}, take the expectation and use the homogeneity relation (4.2) of the random process N, i.e.,

$$\mathbb{E}[\hat{N}(-\boldsymbol{\mu}_2-\mathbf{q}_0)\hat{N}(\mathbf{q})] = (2\pi)^d \hat{R}(\mathbf{q})\,\delta(\mathbf{q}-\boldsymbol{\mu}_2-\mathbf{q}_0).$$

Then upon integration over $\mathbf{q}_0$, I_{11} becomes

$$I_{11} = \frac{1}{\mathrm{i}}\frac{1}{|\mathcal{C}|}\frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{\mu}_1\in\Lambda^*}\int_{\mathcal{C}}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\hat{R}(\mathbf{q})$$

$$\times \sum_{m,n=1}^{2}\frac{1}{(2\pi)^d}\frac{\sum_{m',n'=1}^{2}\sigma_{m'n'}((\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})+(\mathbf{q}-\boldsymbol{\mu}_2))\delta_{n'n}}{E_n((\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})+(\mathbf{q}-\boldsymbol{\mu}_2)) - E_m((\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q}))+\mathrm{i}\theta}$$

$$\times A_{m'm}((\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})+(\mathbf{q}-\boldsymbol{\mu}_2)+\boldsymbol{\mu}_2,(\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q}))$$

$$\times P_{mn}(\mathbf{z},\boldsymbol{\mu}_1,\mathbf{p}-\mathbf{q},(\mathbf{q}-\boldsymbol{\mu}_2))\,\overline{Q_{jl}(\mathbf{z},\boldsymbol{\mu}_1,\mathbf{p})}\,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{z}.$$

Further, by taking into account the orthogonality of the Bloch eigenfunction in P_{mn} and $\overline{Q_{jl}}$, Λ^*-periodicity of $\sigma_{m'n'}$, E_m, and E_n, and summing over $\boldsymbol{\mu}_1,\boldsymbol{\mu}_2\in\Lambda^*$, I_{11} can be simplified to

$$I_{11} = \sum_{m,n=1}^{2}\sum_{m',n'=1}^{2}\frac{1}{\mathrm{i}}\frac{1}{(2\pi)^d}\frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{\mu}\in\Lambda^*}\int_{\mathcal{B}}\hat{R}(\mathbf{q}+\boldsymbol{\mu})\frac{\sigma_{m'n'}(\mathbf{p})\delta_{n'n}\delta_{nl}}{E_n(\mathbf{p})-E_m(\mathbf{p}-\mathbf{q})+\mathrm{i}\theta}$$

$$\times A_{m'm}(\mathbf{p},\mathbf{p}-\mathbf{q}-\boldsymbol{\mu})\,\overline{A_{jm}(\mathbf{p},\mathbf{p}-\mathbf{q}-\boldsymbol{\mu})}\,\mathrm{d}\mathbf{q},$$

where we have used decomposition for $\mathbf{p}\in\mathbb{R}^d$: $\mathbf{p}=\bar{\mathbf{p}}+\bar{\boldsymbol{\mu}}$ with $\bar{\mathbf{p}}\in\mathcal{B}$ and $\bar{\boldsymbol{\mu}}\in\Lambda^*$, and subsequently renamed $\bar{\mathbf{p}}$ and $\bar{\boldsymbol{\mu}}$ back to $\mathbf{p}$ and $\boldsymbol{\mu}$.

For the term I_{12}, we take a similar calculation, i.e., using the relation (4.2) of the random process N,

$$\mathbb{E}[\hat{N}(\mathbf{q}_1)\hat{N}(\mathbf{q})] = (2\pi)^d\hat{R}(\mathbf{q})\,\delta(\mathbf{q}+\mathbf{q}_1)$$

and integrating over $\mathbf{q}_1$, I_{12} becomes

$$I_{12} = \frac{1}{\mathrm{i}}\frac{1}{|\mathcal{C}|}\frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{\mu}_1\in\Lambda^*}\int_{\mathcal{C}}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}R(\mathbf{q})\sum_{m,n=1}^{2}\frac{1}{|\mathcal{B}|}$$

$$\times\int_{\mathcal{B}}\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{z}_1}\frac{\sum_{m',n'=1}^{2}\sigma_{m'n'}(\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})\delta_{m'm}}{E_n((\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})+\mathbf{q}_0)-E_m((\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q}))+\mathrm{i}\theta}$$

$$\times\Psi_n(\mathbf{z}_1,(\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q})+\mathbf{q}_0)\overline{\Psi_{n'}(\mathbf{z}_1,(\mathbf{p}+\boldsymbol{\mu}_1-\mathbf{q}))}\,\mathrm{d}\mathbf{z}_1$$

$$\times P_{mn}(\mathbf{z},\boldsymbol{\mu}_1,\mathbf{p}-\mathbf{q},\mathbf{q}_0)\,\overline{Q_{jl}(\mathbf{z},\boldsymbol{\mu}_1,\mathbf{p})}\,\mathrm{d}\mathbf{q}_0\,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{z},$$

and then, by using the orthogonal property of the Bloch function in P_{mn} and $\overline{Q_{jl}}$,

$$\frac{1}{|\mathcal{B}|}\int_{\mathbb{R}^d}\overline{\Psi_n(\mathbf{z},\mathbf{p}-\mathbf{q}+\mathbf{q}_0)}\,\Psi_l(\mathbf{z},\mathbf{p})\,\mathrm{d}\mathbf{z} = \delta_{nl}\delta_{\mathrm{per}}(-\mathbf{q}+\mathbf{q}_0),$$

we can take the integration over $\mathbf{q}_0$, summation over $\boldsymbol{\mu}_1$, and consider Λ^*-periodicity of $\sigma_{m'n'}$, E_m, and E_n to obtain

$$I_{12} = \frac{1}{\mathrm{i}}\frac{1}{|\mathcal{B}|}\int_{\mathbb{R}^d}R(\mathbf{q})\sum_{m,n=1}^{2}\frac{\sum_{m',n'=1}^{2}\sigma_{m'n'}(\mathbf{p}-\mathbf{q})\delta_{mm'}\delta_{nl}}{E_n(\mathbf{p})-E_m(\mathbf{p}-\mathbf{q})+\mathrm{i}\theta}$$

$$\times\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{z}_1}\Psi_n(\mathbf{z}_1,\mathbf{p})\overline{\Psi_{n'}(\mathbf{z}_1,\mathbf{p}-\mathbf{q})}\,\mathrm{d}\mathbf{z}_1\overline{A_{jm}(\mathbf{p},\mathbf{p}-\mathbf{q})}\,\mathrm{d}\mathbf{q}.$$

Furthermore, by the definition of $A_{nn'}$, we can simplify I_{12} as follows,

$$I_{12} = \sum_{m,n=1}^{2} \sum_{m',n'=1}^{2} \frac{1}{\mathrm{i}} \frac{1}{(2\pi)^d} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu}\in\Lambda^*} \int_{\mathcal{B}} R(\mathbf{q}+\boldsymbol{\mu}) \frac{\sigma_{m'n'}(\mathbf{p}-\mathbf{q})\delta_{mm'}\delta_{nl}}{E_n(\mathbf{p}) - E_m(\mathbf{p}-\mathbf{q}) + \mathrm{i}\theta} \times A_{nn'}(\mathbf{p}, \mathbf{p}-\mathbf{q}-\boldsymbol{\mu}) \overline{A_{jm}(\mathbf{p}, \mathbf{p}-\mathbf{q}-\boldsymbol{\mu})}\, \mathrm{d}\mathbf{q},$$

where we still take the decomposition $\mathbf{p} \in \mathbb{R}^d \mapsto \bar{\mathbf{p}} + \bar{\boldsymbol{\mu}}$ with $\bar{\mathbf{p}} \in \mathcal{B}$ and $\bar{\boldsymbol{\mu}} \in \Lambda^*$, and rename $\bar{\mathbf{p}}, \bar{\boldsymbol{\mu}}$ back into $\mathbf{p}, \boldsymbol{\mu}$.

Thus, combining the simplest forms of I_{11} and I_{12}, we obtain

$$\begin{aligned} I_1 &= I_{11} - I_{12} \\ &= \sum_{m,n=1}^{2} \sum_{m',n'=1}^{2} \frac{1}{\mathrm{i}} \frac{1}{(2\pi)^d} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu}\in\Lambda^*} \int_{\mathcal{B}} \hat{R}(\mathbf{q}+\boldsymbol{\mu}) \frac{\sigma_{m'n'}(\mathbf{p})\delta_{n'n}\delta_{nl}}{E_n(\mathbf{p}) - E_m(\mathbf{p}-\mathbf{q}) + \mathrm{i}\theta} \\ &\quad \times A_{m'm}(\mathbf{p}, \mathbf{p}-\mathbf{q}-\boldsymbol{\mu}) \overline{A_{jm}(\mathbf{p}, \mathbf{p}-\mathbf{q}-\boldsymbol{\mu})}\, \mathrm{d}\mathbf{q} \\ &\quad - \sum_{m,n=1}^{2} \sum_{m',n'=1}^{2} \frac{1}{\mathrm{i}} \frac{1}{(2\pi)^d} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu}\in\Lambda^*} \int_{\mathcal{B}} R(\mathbf{q}+\boldsymbol{\mu}) \frac{\sigma_{m'n'}(\mathbf{p}-\mathbf{q})\delta_{m'm}\delta_{nl}}{E_n(\mathbf{p}) - E_m(\mathbf{p}-\mathbf{q}) + \mathrm{i}\theta} \\ &\quad \times A_{nn'}(\mathbf{p}, \mathbf{p}-\mathbf{q}-\boldsymbol{\mu}) \overline{A_{jm}(\mathbf{p}, \mathbf{p}-\mathbf{q}-\boldsymbol{\mu})}\, \mathrm{d}\mathbf{q} \\ &= \sum_{m,n=1}^{2} \sum_{m',n'=1}^{2} \frac{1}{\mathrm{i}} \frac{1}{(2\pi)^d} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu}\in\Lambda^*} \int_{\mathcal{B}} \frac{\hat{R}(\mathbf{q}+\boldsymbol{\mu})}{E_n(\mathbf{p}) - E_m(\mathbf{p}-\mathbf{q}) + \mathrm{i}\theta} \overline{A_{jm}(\mathbf{p}, \mathbf{p}-\mathbf{q}-\boldsymbol{\mu})} \\ &\quad \times \Big[\sigma_{m'n'}(\mathbf{p})\delta_{n'n}\delta_{nl} A_{m'm}(\mathbf{p}, \mathbf{p}-\mathbf{q}-\boldsymbol{\mu}) - \sigma_{m'n'}(\mathbf{p}-\mathbf{q})\delta_{m'm}\delta_{nl} A_{nn'}(\mathbf{p}, \mathbf{p}-\mathbf{q}-\boldsymbol{\mu})\Big]\, \mathrm{d}\mathbf{q}. \end{aligned}$$

Similarly to [3], one can verify $I_2 = \overline{I_1}$. Therefore, by taking the limit $\theta \to 0$ and the change of variable $\mathbf{q} \mapsto \mathbf{p} - \mathbf{q}$, the R.H.S finally becomes

(4.14)

$$\begin{aligned} &\text{R.H.S} \\ &= \sum_{m,n=1}^{2} \sum_{m',n'=1}^{2} \frac{1}{(2\pi)^{d-1}} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu}\in\Lambda^*} \int_{\mathcal{B}} \hat{R}(\mathbf{p}-\mathbf{q}+\boldsymbol{\mu}) \delta(E_n(\mathbf{p}) - E_m(\mathbf{q})) \overline{A_{jm}(\mathbf{p}, \mathbf{q}-\boldsymbol{\mu})} \\ &\quad \times \Big[\sigma_{m'n'}(\mathbf{q})\delta_{m'm}\delta_{nl} A_{nn'}(\mathbf{p}, \mathbf{q}-\boldsymbol{\mu}) - \sigma_{m'n'}(\mathbf{p})\delta_{n'n}\delta_{nl} A_{m'm}(\mathbf{p}, \mathbf{q}-\boldsymbol{\mu})\Big]\, \mathrm{d}\mathbf{q} \\ &\quad + \frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p}) - E_j(\mathbf{p})]\sigma_{jl} \\ &= \sum_{m,n=1}^{2} \sum_{m',n'=1}^{2} \frac{1}{(2\pi)^{d-1}} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu}\in\Lambda^*} \int_{\mathcal{B}} \hat{R}(\mathbf{p}-\mathbf{q}+\boldsymbol{\mu}) \delta(E_l(\mathbf{p}) - E_m(\mathbf{q})) \overline{A_{jm}(\mathbf{p}, \mathbf{q}-\boldsymbol{\mu})} \\ &\quad \times \Big[\sigma_{mn'}(\mathbf{q}) A_{ln'}(\mathbf{p}, \mathbf{q}-\boldsymbol{\mu}) - \sigma_{m'l}(\mathbf{p}) A_{m'm}(\mathbf{p}, \mathbf{q}-\boldsymbol{\mu})\Big]\, \mathrm{d}\mathbf{q} \\ &\quad + \frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p}) - E_j(\mathbf{p})]\sigma_{jl} \\ &= \sum_{m=1}^{2} \sum_{m'=1}^{2} \frac{1}{(2\pi)^{d-1}} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu}\in\Lambda^*} \int_{\mathcal{B}} \hat{R}(\mathbf{p}-\mathbf{q}+\boldsymbol{\mu}) \delta(E_l(\mathbf{p}) - E_m(\mathbf{q})) \overline{A_{jm}(\mathbf{p}, \mathbf{q}-\boldsymbol{\mu})} \\ &\quad \times \Big[\sigma_{mm'}(\mathbf{q}) A_{lm'}(\mathbf{p}, \mathbf{q}-\boldsymbol{\mu}) - \sigma_{m'l}(\mathbf{p}) A_{m'm}(\mathbf{p}, \mathbf{q}-\boldsymbol{\mu})\Big]\, \mathrm{d}\mathbf{q} \\ &\quad + \frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p}) - E_j(\mathbf{p})]\sigma_{jl}, \quad j, l \in \{1, 2\}, \end{aligned}$$

where repeated indexes are removed in the last equality above.

Thus, focusing on the $O(1)$ term and combining the L.H.S in (4.13) and R.H.S in (4.14), we finally obtain the following coupled system:

(4.15)
$$\begin{aligned}&\partial_t\sigma_{jl}(t,\mathbf{x},\mathbf{p})+\sum_{n=1}^{2}\nabla_{\mathbf{x}}\sigma_{jn}(t,\mathbf{x},\mathbf{p})\cdot\langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_l,\Psi_n\rangle_{\mathcal{C}}\\&\quad=\sum_{m=1}^{2}\sum_{m'=1}^{2}\frac{1}{(2\pi)^{d-1}}\frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{\mu}\in\Lambda^*}\int_{\mathcal{B}}\hat{R}(\mathbf{p}-\mathbf{q}+\boldsymbol{\mu})\delta(E_l(\mathbf{p})-E_m(\mathbf{q}))\overline{A_{jm}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})}\\&\qquad\times\Big[\sigma_{mm'}(\mathbf{q})A_{lm'}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})-\sigma_{m'l}(\mathbf{p})A_{m'm}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})\Big]\,\mathrm{d}\mathbf{q}\\&\qquad+\frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p})-E_j(\mathbf{p})]\sigma_{jl},\quad j,l\in\{1,2\}.\end{aligned}$$

Note that the discussion of section 3.2 in the deterministic case also applies to the model (4.15). More specifically, if we take the transformation (3.18), we can obtain the coupled system for $\widetilde{\sigma}_{jl}$ by involving the phase factors as follows:

(4.16)
$$\begin{aligned}&\partial_t\widetilde{\sigma}_{jl}(t,\mathbf{x},\mathbf{p})+\sum_{n=1}^{2}\nabla_{\mathbf{x}}\widetilde{\sigma}_{jn}(t,\mathbf{x},\mathbf{p})\cdot\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p})-E_n(\mathbf{p})]t}\langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_l,\Psi_n\rangle_{\mathcal{C}}\\&\quad=\sum_{m=1}^{2}\sum_{m'=1}^{2}\frac{1}{(2\pi)^{d-1}}\frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{\mu}\in\Lambda^*}\int_{\mathcal{B}}\hat{R}(\mathbf{p}-\mathbf{q}+\boldsymbol{\mu})\delta(E_l(\mathbf{p})-E_m(\mathbf{q}))\overline{A_{jm}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})}\\&\qquad\times\Big[\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}[E_m(\mathbf{q})-E_{m'}(\mathbf{q})+E_l(\mathbf{p})-E_j(\mathbf{p})]t}\widetilde{\sigma}_{mm'}(\mathbf{q})A_{lm'}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})\\&\qquad-\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}[E_{m'}(\mathbf{p})-E_j(\mathbf{p})]t}\widetilde{\sigma}_{m'l}(\mathbf{p})A_{m'm}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})\Big]\,\mathrm{d}\mathbf{q}.\end{aligned}$$

Similar calculations as in section 3.2 then show that, for $\mathbf{p}$ sufficiently far away from band crossings, the system (4.16) reduces to [3, eq. (3.15)] for the diagonal σ's, σ_{jj}, $j\in\{1,2\}$, while the off-diagonal σ's, σ_{jl}, $j\neq l$, can be neglected because if they are initially zero, they remain zero for all t. We provide these calculations in Appendix C. In the following section we focus on the dynamics of the system (4.15) close to band crossings in the particular case of graphene.

5. Application: Effective dynamics of wave packets in graphene with randomness. In this section we will specialize the model (4.15) derived in the previous section to the particular case of the Schrödinger operator with a honeycomb potential, modeling the dynamics of the wave function of an electron in graphene.

We start by reviewing the important features of the band structure of such operators, following [19, 20, 9]. Generically, with respect to the magnitude of the potential [19], we may assume that two bands are degenerate at the so-called Dirac points in the Brillouin zone. These points are generally denoted by $\mathbf{K}$ and $\mathbf{K}':=-\mathbf{K}$; see Figure 2. Nearby to these points, the dispersion surface is conical, i.e.,

(5.1)
$$E_1(\mathbf{p})=-\lambda_\sharp|\mathbf{p}-\mathbf{K}|+o(|\mathbf{p}-\mathbf{K}|),\quad E_2(\mathbf{p})=\lambda_\sharp|\mathbf{p}-\mathbf{K}|+o(|\mathbf{p}-\mathbf{K}|),\quad \mathbf{p}\to\mathbf{K},$$

where $\lambda_\sharp$ is a positive constant known as the Fermi velocity [37, 19]. In what follows we assume further that the bands E_1,E_2 are otherwise separated, as happens for

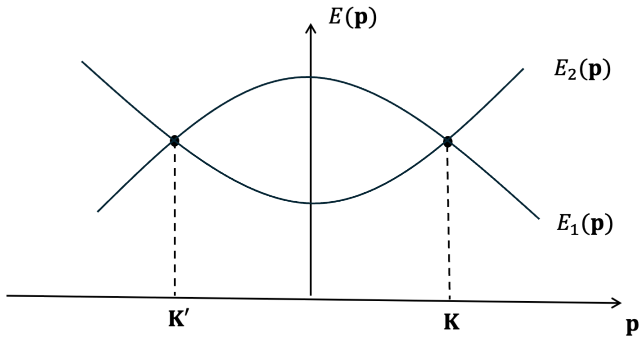

FIG. 2. *Schematic of energy band crossings for graphene.*

tight-binding models [37]. In this case (5.1) describes the shape of the bands as they intersect the Fermi level, which we take to be the zero of energy for convenience. To our knowledge, it is not known whether other eigenvalues can coincide with the Dirac energy for the full PDE model of graphene [19].

Recalling the discussion of different regimes in section 3.2, here we consider more precisely the case where $|\mathbf{p}-\mathbf{K}| = O(\varepsilon)$ or $|\mathbf{p}-\mathbf{K}'| = O(\varepsilon)$. This is the regime considered in [20], where ε corresponds to the wave-packet width in momentum space, and should be the one relevant for the physics of graphene for temperatures T so that $k_B T \ll E$, where $k_B \approx 8.6 \times 10^{-5}\ eV K^{-1}$ is Planck's constant and $E \approx 2.6\ eV$ is the graphene bandwidth energy scale. Note that this holds even at room temperature $T \approx 300\ K$. In the opposite case, where $|\mathbf{p}-\mathbf{K}| \gg \varepsilon$ and $|\mathbf{p}-\mathbf{K}'| \gg \varepsilon$, the system (4.15) reduces to the result of Bal et al. [3] as explained in Appendix C.

Assuming $|\mathbf{p}-\mathbf{K}| = O(\varepsilon)$ (the case $|\mathbf{p} = \mathbf{K}'| = O(\varepsilon)$ is similar), we can obtain a closed system for σ's with momenta near to the Dirac points by observing that, under our assumptions on the graphene band structure near to 0 energy, the $\delta(E_l(\mathbf{p}) - E_m(\mathbf{q}))$ appearing in (4.15) can be nonzero only for $|\mathbf{q}-\mathbf{K}| = O(\varepsilon)$ or $|\mathbf{q}-\mathbf{K}'| = O(\varepsilon)$. We can then replace (4.15) by the simplified system

(5.2)

$$\partial_t \sigma_{jl}(t,\mathbf{x},\mathbf{p}) + \sum_{n=1}^{2} \nabla_{\mathbf{x}} \sigma_{jn}(t,\mathbf{x},\mathbf{p}) \cdot \langle (-\mathrm{i}\nabla_{\mathbf{z}})\Psi_l(\cdot,\mathbf{p}), \Psi_n(\cdot,\mathbf{p})\rangle_{\mathcal{C}}$$

$$= \sum_{m=1}^{2}\sum_{m'=1}^{2} \frac{1}{(2\pi)^{d-1}} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu}\in\Lambda^*} \int_{\mathcal{B}_\varepsilon(\mathbf{K},\mathbf{K}')} \hat{R}(\mathbf{p}-\mathbf{q}+\boldsymbol{\mu})\delta(E_l(\mathbf{p})-E_m(\mathbf{q}))\overline{A_{jm}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})}$$

$$\times \Big[\sigma_{mm'}(\mathbf{q})A_{lm'}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu}) - \sigma_{m'l}(\mathbf{p})A_{m'm}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})\Big]\,\mathrm{d}\mathbf{q} + \frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p}) - E_j(\mathbf{p})]\sigma_{jl},$$

where $\mathcal{B}_\varepsilon(\mathbf{K},\mathbf{K}')$ denotes the union of balls with radius proportional to ε centered at $\mathbf{K}$ and $\mathbf{K}'$. Note that the system (5.2) couples only σ's with momenta near to $\mathbf{K}$ and $\mathbf{K}'$, and that the final relaxation term in (5.2) is $O(1)$ as $\varepsilon \downarrow 0$ by our assumptions on $\mathbf{p}$ and (5.1). We can interpret (5.2) as describing the evolution of wave packets concentrated at Dirac points $\mathbf{K}$ and $\mathbf{K}'$ with momentum width ε coupled to each other by the random potential.

Further simplifications are possible if we assume that $|\mathbf{p}-\mathbf{K}| = o(\varepsilon)$ or $|\mathbf{p}-\mathbf{K}'| = o(\varepsilon)$. In this case, after dropping higher-order terms, we can obtain a closed system for $\sigma_{jl}(t,\mathbf{x},\mathbf{p})$ for $\mathbf{p} \in \{\mathbf{K},\mathbf{K}'\}$ as

$$
\begin{aligned}
&\partial_t \sigma_{jl}(t,\mathbf{x},\mathbf{K}) + \sum_{n=1}^{2} \nabla_{\mathbf{x}} \sigma_{jn}(t,\mathbf{x},\mathbf{K}) \cdot \langle (-\mathrm{i}\nabla_{\mathbf{z}})\Psi_l(\cdot,\mathbf{K}), \Psi_n(\cdot,\mathbf{K})\rangle_{\mathcal{C}} \\
&= \sum_{m=1}^{2}\sum_{m'=1}^{2} \frac{1}{(2\pi)^{d-1}} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu}\in\Lambda^*} \sum_{\mathbf{q}=\mathbf{K},\mathbf{K}'} \hat{R}(\mathbf{K}-\mathbf{q}+\boldsymbol{\mu}) \overline{A_{jm}(\mathbf{K},\mathbf{q}-\boldsymbol{\mu})} \\
&\quad \times \Big[\sigma_{mm'}(\mathbf{q}) A_{lm'}(\mathbf{K},\mathbf{q}-\boldsymbol{\mu}) - \sigma_{m'l}(\mathbf{K}) A_{m'm}(\mathbf{K},\mathbf{q}-\boldsymbol{\mu}) \Big]
\end{aligned} \tag{5.3}
$$

and

$$
\begin{aligned}
&\partial_t \sigma_{jl}(t,\mathbf{x},\mathbf{K}') + \sum_{n=1}^{2} \nabla_{\mathbf{x}} \sigma_{jn}(t,\mathbf{x},\mathbf{K}') \cdot \langle (-\mathrm{i}\nabla_{\mathbf{z}})\Psi_l(\cdot,\mathbf{K}'), \Psi_n(\cdot,\mathbf{K}')\rangle_{\mathcal{C}} \\
&= \sum_{m=1}^{2}\sum_{m'=1}^{2} \frac{1}{(2\pi)^{d-1}} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu}\in\Lambda^*} \sum_{\mathbf{q}=\mathbf{K},\mathbf{K}'} \hat{R}(\mathbf{K}'-\mathbf{q}+\boldsymbol{\mu}) \overline{A_{jm}(\mathbf{K}',\mathbf{q}-\boldsymbol{\mu})} \\
&\quad \times \Big[\sigma_{mm'}(\mathbf{q}) A_{lm'}(\mathbf{K}',\mathbf{q}-\boldsymbol{\mu}) - \sigma_{m'l}(\mathbf{K}') A_{m'm}(\mathbf{K}',\mathbf{q}-\boldsymbol{\mu}) \Big].
\end{aligned} \tag{5.4}
$$

Note that the off-diagonal σ's cannot be ignored in either of the systems (5.2) or (5.3)–(5.4).

To our knowledge, the models (5.2) or (5.3)–(5.4) are original to the present work. They are straightforward to interpret: in the presence of a weak random potential as in (4.1), wave packets concentrated at the Dirac points in graphene no longer satisfy independent dynamics but become coupled. A similar model, where wave-packets propagating along domain walls in modulated graphene-like structures can become "valley-coupled" through a random perturbation, was recently introduced in [2]. Note that the shape of the eigenvalue bands at the crossing, which is linear in graphene ($r=1$ in (3.21)), determines the regime where the reduced models we derive are valid. In the case of a crossing where $r\neq 1$, the regime would have to be modified from $|\mathbf{p}-\mathbf{K}| = O(\varepsilon)$ to $|\mathbf{p}-\mathbf{K}| = O(\varepsilon^{1/r})$.

6. Conclusions. In this paper, we investigate the semiclassical limit of the Schrödinger equation featuring general periodic potentials across arbitrary dimensions. Our focus lies on situations where energy bands exhibit crossings, a characteristic particularly significant for materials such as graphene. In the absence of randomness, we develop a coupled Liouville system with a relaxation-type source term, capturing the interplay between energy bands. Conversely, when introducing random perturbations, we establish a coupled radiative transport system. Here, an additional collision-like term elucidates interactions between distinct wave vectors sharing the same energy. As a special case, we examine the potential of a honeycomb structure. Our newly derived system unveils that for wave packets concentrated at the Dirac points in graphene, they no longer exhibit independent dynamics but rather become coupled.

Appendix A. Derivation of orthogonality relation. In this section, we present the complete derivation of the orthogonality (3.12). For $\mathbf{p}\in\mathcal{B}$, we have

$$
\begin{aligned}
&\langle Q_{mn}(\cdot,\cdot,\mathbf{p}), Q_{jl}(\cdot,\cdot,\mathbf{p})\rangle_{\mathcal{C},\Lambda^*} \\
&\quad = \sum_{\boldsymbol{\mu}\in\Lambda^*} \frac{1}{|\mathcal{C}|} \int_{\mathcal{C}} Q_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p}) \overline{Q_{jl}(\mathbf{z},\boldsymbol{\mu},\mathbf{p})}\,\mathrm{d}\mathbf{z} \\
&\quad = \sum_{\boldsymbol{\mu}\in\Lambda^*} \int_{\mathcal{C}} \frac{1}{|\mathcal{C}|} \left[\int_{\mathcal{C}} \frac{1}{|\mathcal{C}|} \mathrm{e}^{\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot\mathbf{y}} \Psi_m(\mathbf{z}-\mathbf{y},\mathbf{p}) \overline{\Psi_n(\mathbf{z},\mathbf{p})}\,\mathrm{d}\mathbf{y} \right]
\end{aligned} \tag{A.1}
$$

$$\times\left[\int_{\mathcal{C}}\frac{1}{|\mathcal{C}|}\,\mathrm{e}^{-\,\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot\mathbf{y}'}\overline{\Psi_j(\mathbf{z}-\mathbf{y}',\mathbf{p})}\Psi_l(\mathbf{z},\mathbf{p})\,\mathrm{d}\mathbf{y}'\right]\mathrm{d}\mathbf{z}$$
$$=\sum_{\boldsymbol{\mu}\in\Lambda^*}\int_{\mathcal{C}}\frac{1}{|\mathcal{C}|}\left[\int_{\mathcal{C}'}\frac{1}{|\mathcal{C}|}\,\mathrm{e}^{\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot(\mathbf{z}-\mathbf{y})}\Psi_m(\mathbf{y},\mathbf{p})\overline{\Psi_n(\mathbf{z},\mathbf{p})}\,\mathrm{d}\mathbf{y}\right]$$
$$\times\left[\int_{\mathcal{C}'}\frac{1}{|\mathcal{C}|}\,\mathrm{e}^{-\,\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot(\mathbf{z}-\mathbf{y}')}\overline{\Psi_j(\mathbf{y}',\mathbf{p})}\Psi_l(\mathbf{z},\mathbf{p})\,\mathrm{d}\mathbf{y}'\right]\mathrm{d}\mathbf{z},$$

where we applied the change of variables

$$\mathbf{y}\mapsto(\mathbf{z}-\mathbf{y}),\qquad \mathbf{y}'\mapsto(\mathbf{z}-\mathbf{y}')$$

with the change of domain $\mathcal{C}\mapsto\mathcal{C}'$ in the last equality above. By further integrating over $\mathbf{z}$ and using the relation

$$\frac{1}{|\mathcal{C}|}\int_{\mathcal{C}}\overline{\Psi_n(\mathbf{z},\mathbf{p})}\,\Psi_l(\mathbf{z},\mathbf{p})\,\mathrm{d}\mathbf{z}=\delta_{ln}$$

(A.1) becomes

(A.2)
$$\delta_{ln}\frac{1}{|\mathcal{C}|}\sum_{\boldsymbol{\mu}\in\Lambda^*}\int_{\mathcal{C}'}\int_{\mathcal{C}'}\frac{1}{|\mathcal{C}|}\,\mathrm{e}^{\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot(\mathbf{y}'-\mathbf{y})}\Psi_m(\mathbf{y},\mathbf{p})\,\overline{\Psi_j(\mathbf{y}',\mathbf{p})}\,\mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{y}'$$
$$=\delta_{ln}\int_{\mathcal{C}'}\int_{\mathcal{C}'}\frac{1}{|\mathcal{C}|}\sum_{\boldsymbol{\nu}\in\Lambda}\delta((\mathbf{y}'-\mathbf{y})-\boldsymbol{\nu})\,\mathrm{e}^{\mathrm{i}\mathbf{p}(\mathbf{y}'-\mathbf{y})}\Psi_m(\mathbf{y},\mathbf{p})\,\overline{\Psi_j(\mathbf{y}',\mathbf{p})}\,\mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{y}'$$
$$=\delta_{ln}\int_{\mathcal{C}'}\int_{\mathcal{C}'}\frac{1}{|\mathcal{C}|}\sum_{\boldsymbol{\nu}\in\Lambda}\delta((\mathbf{y}'-\mathbf{y})-\boldsymbol{\nu})\,\mathrm{e}^{\mathrm{i}\mathbf{p}(\mathbf{y}'-\mathbf{y})}\Psi_m(\mathbf{y},\mathbf{p})\,\overline{\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\boldsymbol{\nu}}\Psi_j(\mathbf{y}'-\boldsymbol{\nu},\mathbf{p})}\,\mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{y}'$$
$$=\delta_{ln}\int_{\mathcal{C}'}\int_{\mathcal{C}'}\frac{1}{|\mathcal{C}|}\sum_{\boldsymbol{\nu}\in\Lambda}\delta((\mathbf{y}'-\mathbf{y})-\boldsymbol{\nu})\,\mathrm{e}^{\mathrm{i}\mathbf{p}(\mathbf{y}'-\boldsymbol{\nu}-\mathbf{y})}\Psi_m(\mathbf{y},\mathbf{p})\,\overline{\Psi_j(\mathbf{y}'-\boldsymbol{\nu},\mathbf{p})}\,\mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{y}'$$
$$=\delta_{ln}\int_{\mathcal{C}'}\frac{1}{|\mathcal{C}|}\Psi_m(\mathbf{y},\mathbf{p})\,\overline{\Psi_j(\mathbf{y},\mathbf{p})}\,\mathrm{d}\mathbf{y}$$
$$=\delta_{ln}\delta_{jm},$$

where we use the following identity [43, Appendix A] in the first equality above,

(A.3)
$$\frac{1}{|\mathcal{C}|}\sum_{\boldsymbol{\mu}\in\Lambda^*}\mathrm{e}^{\mathrm{i}\boldsymbol{\mu}\cdot\mathbf{z}}=\sum_{\boldsymbol{\nu}\in\Lambda}\delta(\mathbf{z}-\boldsymbol{\nu})\Rightarrow\frac{1}{|\mathcal{C}|}\sum_{\boldsymbol{\mu}\in\Lambda^*}\mathrm{e}^{\mathrm{i}\boldsymbol{\mu}\cdot(\mathbf{y}'-\mathbf{y})}=\sum_{\boldsymbol{\nu}\in\Lambda}\delta(\mathbf{y}'-\mathbf{y}-\boldsymbol{\nu}),$$

and the periodicity of Bloch eigenfunction $(2.1)_2$ in the second equality.

By involving the integration by parts and product rule, it then yields (3.13) and (3.14) by following similar calculations, respectively.

Appendix B. Derivation of $\boldsymbol{\eta_{jl}}$. In this section, we provide the specific calculation process of η_{jl}, i.e., from (4.10) to (4.11). To clarify, we first present the derivation of (I) in (4.11):

$$(I)=\frac{1}{(2\pi)^d}\frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{\mu}\in\Lambda^*}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\hat{N}(\mathbf{q})W_0(\mathbf{z},\mathbf{p}+\boldsymbol{\mu}-\mathbf{q})\,\overline{P_{jl}(\mathbf{z},\boldsymbol{\mu},\mathbf{p},\mathbf{q}_0)}\,\mathrm{d}\mathbf{z}\,\mathrm{d}\mathbf{q}$$
$$=\frac{1}{(2\pi)^d}\frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{\mu}\in\Lambda^*}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\hat{N}(\mathbf{q})\left[\sum_{m,n=1}^{2}\sigma_{mn}(t,\mathbf{x},\mathbf{p}-\mathbf{q})Q_{mn}(\mathbf{z},\boldsymbol{\mu},\mathbf{p}-\mathbf{q})\right]$$

$$
\begin{aligned}
&\times \frac{1}{|\mathcal{C}|}\int_{\mathcal{C}} \mathrm{e}^{-\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot\mathbf{y}_2}\overline{\Psi_j(\mathbf{z}-\mathbf{y}_2,\mathbf{p})}\,\Psi_l(\mathbf{z},\mathbf{p}+\mathbf{q}_0)\,\mathrm{d}\mathbf{y}_2\,\mathrm{d}\mathbf{z}\,\mathrm{d}\mathbf{q}\\
&= \frac{1}{(2\pi)^d}\frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{\mu}\in\Lambda^*}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\hat{N}(\mathbf{q})\\
&\times\left[\sum_{m,n=1}^{2}\sigma_{mn}(t,\mathbf{x},\mathbf{p}-\mathbf{q})\frac{1}{|\mathcal{C}|}\int_{\mathcal{C}}\mathrm{e}^{\mathrm{i}(\mathbf{p}+\boldsymbol{\mu}-\mathbf{q})\cdot\mathbf{y}_1}\Psi_m(\mathbf{z}-\mathbf{y}_1,\mathbf{p}-\mathbf{q})\,\overline{\Psi_n(\mathbf{z},\mathbf{p}-\mathbf{q})}\,\mathrm{d}\mathbf{y}_1\right]\\
&\times \frac{1}{|\mathcal{C}|}\int_{\mathcal{C}} \mathrm{e}^{-\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot\mathbf{y}_2}\overline{\Psi_j(\mathbf{z}-\mathbf{y}_2,\mathbf{p})}\,\Psi_l(\mathbf{z},\mathbf{p}+\mathbf{q}_0)\,\mathrm{d}\mathbf{y}_2\,\mathrm{d}\mathbf{z}\,\mathrm{d}\mathbf{q}.
\end{aligned}
$$

By using the following change of variables:

$$
\mathbf{y}_1\mapsto\mathbf{z}-\mathbf{y}_1\qquad \mathbf{y}_2\mapsto\mathbf{z}-\mathbf{y}_2,
$$

it yields that

$$
\begin{aligned}
(I) &= \frac{1}{(2\pi)^d}\frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{\mu}\in\Lambda^*}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\hat{N}(\mathbf{q})\sum_{m,n=1}^{2}\sigma_{mn}(t,\mathbf{x},\mathbf{p}-\mathbf{q})\\
&\times\frac{1}{|\mathcal{C}|^2}\int_{\mathcal{C}'\times\mathcal{C}'}\mathrm{e}^{\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot(\mathbf{y}_2-\mathbf{y}_1)}\,\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{y}_1}\Psi_m(\mathbf{y}_1,\mathbf{p}-\mathbf{q})\,\overline{\Psi_j(\mathbf{y}_2,\mathbf{p})}\\
&\times\Psi_l(\mathbf{z},\mathbf{p}+\mathbf{q}_0)\,\overline{\Psi_n(\mathbf{z},\mathbf{p}-\mathbf{q})}\,\mathrm{d}\mathbf{y}_1\,\mathrm{d}\mathbf{y}_2\,\mathrm{d}\mathbf{z}\,\mathrm{d}\mathbf{q}\\
&= \frac{1}{(2\pi)^d}\sum_{\boldsymbol{\mu}\in\Lambda^*}\int_{\mathbb{R}^d}\hat{N}(\mathbf{q})\sum_{m,n=1}^{2}\sigma_{mn}(t,\mathbf{x},\mathbf{p}-\mathbf{q})\delta_{nl}\delta_{\mathrm{per}}(-\mathbf{q}-\mathbf{q}_0)\\
&\times\frac{1}{|\mathcal{C}|^2}\int_{\mathcal{C}'\times\mathcal{C}'}\mathrm{e}^{\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot(\mathbf{y}_2-\mathbf{y}_1)}\,\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{y}_1}\Psi_m(\mathbf{y}_1,\mathbf{p}-\mathbf{q})\,\overline{\Psi_j(\mathbf{y}_2,\mathbf{p})}\,\mathrm{d}\mathbf{y}_1\,\mathrm{d}\mathbf{y}_2\,\mathrm{d}\mathbf{q},
\end{aligned}
$$

where the orthogonality (2.4) is used in the last equality.

Taking another change of variable

$$
\mathbf{q}\mapsto\bar{\mathbf{q}}-\bar{\boldsymbol{\mu}}\quad\text{with}\quad \mathbf{q}\in\mathbb{R}^d,\quad \bar{\mathbf{q}}\in\mathcal{B},\quad \bar{\boldsymbol{\mu}}\in\Lambda^*,
$$

$$
\begin{aligned}
(I) &= \frac{1}{(2\pi)^d}\sum_{\boldsymbol{\mu}\in\Lambda^*}\sum_{\bar{\boldsymbol{\mu}}\in\Lambda^*}\int_{\mathcal{B}}\hat{N}(\bar{\mathbf{q}}-\bar{\boldsymbol{\mu}})\sum_{m,n=1}^{2}\sigma_{mn}(t,\mathbf{x},\mathbf{p}-(\bar{\mathbf{q}}-\bar{\boldsymbol{\mu}}))\delta_{nl}\\
&\times\frac{1}{|\mathcal{C}|^2}\int_{\mathcal{C}'\times\mathcal{C}'}\mathrm{e}^{\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot(\mathbf{y}_2-\mathbf{y}_1)}\,\mathrm{e}^{\mathrm{i}(\bar{\mathbf{q}}-\bar{\boldsymbol{\mu}})\cdot\mathbf{y}_1}\Psi_m(\mathbf{y}_1,\mathbf{p}-(\bar{\mathbf{q}}-\bar{\boldsymbol{\mu}}))\overline{\Psi_j(\mathbf{y}_2,\mathbf{p})}\\
&\times\delta_{\mathrm{per}}(-(\bar{\mathbf{q}}-\bar{\boldsymbol{\mu}})-\mathbf{q}_0)\,\mathrm{d}\mathbf{y}_1\,\mathrm{d}\mathbf{y}_2\,\mathrm{d}\bar{\mathbf{q}}\\
&= \frac{1}{(2\pi)^d}\sum_{\boldsymbol{\mu}\in\Lambda^*}\sum_{\bar{\boldsymbol{\mu}}\in\Lambda^*}\int_{\mathcal{B}}\hat{N}(\bar{\mathbf{q}}-\bar{\boldsymbol{\mu}})\sum_{m,n=1}^{2}\sigma_{mn}(t,\mathbf{x},\mathbf{p}-\bar{\mathbf{q}})\delta_{nl}\\
&\times\frac{1}{|\mathcal{C}|^2}\int_{\mathcal{C}'\times\mathcal{C}'}\mathrm{e}^{\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot(\mathbf{y}_2-\mathbf{y}_1)}\,\mathrm{e}^{\mathrm{i}(\bar{\mathbf{q}}-\bar{\boldsymbol{\mu}})\cdot\mathbf{y}_1}\Psi_m(\mathbf{y}_1,\mathbf{p}-(\bar{\mathbf{q}}-\bar{\boldsymbol{\mu}}))\,\overline{\Psi_j(\mathbf{y}_2,\mathbf{p})}\\
&\times\delta_{\mathrm{per}}(-\bar{\mathbf{q}}-\mathbf{q}_0)\,\mathrm{d}\mathbf{y}_1\,\mathrm{d}\mathbf{y}_2\,\mathrm{d}\bar{\mathbf{q}}\\
&= \frac{1}{(2\pi)^d}\sum_{\boldsymbol{\mu}\in\Lambda^*}\sum_{\bar{\boldsymbol{\mu}}\in\Lambda^*}\hat{N}(-\mathbf{q}_0-\bar{\boldsymbol{\mu}})\sum_{m,n=1}^{2}\sigma_{mn}(t,\mathbf{x},\mathbf{p}+\mathbf{q}_0)\delta_{nl}\\
&\times\frac{1}{|\mathcal{C}|^2}\int_{\mathcal{C}'\times\mathcal{C}'}\mathrm{e}^{\mathrm{i}(\mathbf{p}+\boldsymbol{\mu})\cdot(\mathbf{y}_2-\mathbf{y}_1)}\,\mathrm{e}^{\mathrm{i}(-\mathbf{q}_0-\bar{\boldsymbol{\mu}})\cdot\mathbf{y}_1}\Psi_m(\mathbf{y}_1,\mathbf{p}-(-\mathbf{q}_0-\bar{\boldsymbol{\mu}}))\,\overline{\Psi_j(\mathbf{y}_2,\mathbf{p})}\,\mathrm{d}\mathbf{y}_1\,\mathrm{d}\mathbf{y}_2
\end{aligned}
$$

$$
\begin{aligned}
&\times \frac{1}{(2\pi)^d} \sum_{\bar{\boldsymbol{\mu}} \in \Lambda^*} \hat{N}(-\mathbf{q}_0 - \bar{\boldsymbol{\mu}}) \sum_{m,n=1}^{2} \sigma_{mn}(t, \mathbf{x}, \mathbf{p} + \mathbf{q}_0) \delta_{nl} \\
&\times \frac{1}{|\mathcal{C}|} \int_{\mathcal{C}' \times \mathcal{C}'} \mathrm{e}^{\mathrm{i}\mathbf{p} \cdot (\mathbf{y}_2 - \mathbf{y}_1)} \, \mathrm{e}^{\mathrm{i}(-\mathbf{q}_0 - \bar{\boldsymbol{\mu}}) \cdot \mathbf{y}_1} \Psi_m(\mathbf{y}_1, \mathbf{p} - (-\mathbf{q}_0 - \bar{\boldsymbol{\mu}})) \\
&\times \overline{\Psi_j(\mathbf{y}_2, \mathbf{p})} \sum_{\boldsymbol{\nu} \in \Lambda} \delta(\mathbf{y}_2 - \mathbf{y}_1 - \boldsymbol{\nu}) \, \mathrm{d}\mathbf{y}_1 \, \mathrm{d}\mathbf{y}_2 \\
= &\frac{1}{(2\pi)^d} \sum_{\bar{\boldsymbol{\mu}} \in \Lambda^*} \hat{N}(-\mathbf{q}_0 - \bar{\boldsymbol{\mu}}) \sum_{m,n=1}^{2} \sigma_{mn}(t, \mathbf{x}, \mathbf{p} + \mathbf{q}_0) \delta_{nl} \\
&\times \frac{1}{|\mathcal{C}|} \int_{\mathcal{C}' \times \mathcal{C}'} \mathrm{e}^{\mathrm{i}\mathbf{p} \cdot (\mathbf{y}_2 - \boldsymbol{\nu} - \mathbf{y}_1)} \, \mathrm{e}^{\mathrm{i}(-\mathbf{q}_0 - \bar{\boldsymbol{\mu}}) \cdot \mathbf{y}_1} \Psi_m(\mathbf{y}_1, \mathbf{p} - (-\mathbf{q}_0 - \bar{\boldsymbol{\mu}})) \\
&\times \overline{\Psi_j(\mathbf{y}_2 - \boldsymbol{\nu}, \mathbf{p})} \sum_{\boldsymbol{\nu} \in \Lambda} \delta(\mathbf{y}_2 - \mathbf{y}_1 - \boldsymbol{\nu}) \, \mathrm{d}\mathbf{y}_1 \, \mathrm{d}\mathbf{y}_2 \\
= &\frac{1}{(2\pi)^d} \sum_{\bar{\boldsymbol{\mu}} \in \Lambda^*} \hat{N}(-\mathbf{q}_0 - \bar{\boldsymbol{\mu}}) \sum_{m,n=1}^{2} \sigma_{mn}(t, \mathbf{x}, \mathbf{p} + \mathbf{q}_0) \delta_{nl} \\
&\times \frac{1}{|\mathcal{C}|} \int_{\mathcal{C}'} \mathrm{e}^{-\mathrm{i}(\mathbf{q}_0 + \bar{\boldsymbol{\mu}}) \cdot \mathbf{y}_1} \Psi_m(\mathbf{y}_1, \mathbf{p} + \mathbf{q}_0 + \bar{\boldsymbol{\mu}}) \overline{\Psi_j(\mathbf{y}_1, \mathbf{p})} \, \mathrm{d}\mathbf{y}_1 \\
= &\frac{1}{(2\pi)^d} \sum_{\boldsymbol{\mu} \in \Lambda^*} \hat{N}(-\mathbf{q}_0 - \boldsymbol{\mu}) \sum_{m,n=1}^{2} \sigma_{mn}(t, \mathbf{x}, \mathbf{p} + \mathbf{q}_0) \delta_{nl} \\
&\times \underbrace{\frac{1}{|\mathcal{C}|} \int_{\mathcal{C}'} \mathrm{e}^{-\mathrm{i}(\mathbf{q}_0 + \boldsymbol{\mu}) \cdot \mathbf{y}} \Psi_m(\mathbf{y}, \mathbf{p} + \mathbf{q}_0 + \boldsymbol{\mu}) \, \overline{\Psi_j(\mathbf{y}, \mathbf{p})} \, \mathrm{d}\mathbf{y},}_{:= A_{mj}(\mathbf{p} + \mathbf{q}_0 + \boldsymbol{\mu}, \mathbf{p})}
\end{aligned}
$$

where we consider the Λ^*-periodic σ_{mn} in the second equality above and rename $\mathbf{y}_1 \mapsto \mathbf{y}$ and $\bar{\boldsymbol{\mu}} \mapsto \boldsymbol{\mu}$ in the last equality above.

To derive the term (II) of (4.11), we start with

$$
\begin{aligned}
(II) = &\frac{1}{(2\pi)^d} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu} \in \Lambda^*} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\mathbf{q} \cdot \mathbf{z}} \hat{N}(\mathbf{q}) W_0(\mathbf{z}, \mathbf{p} + \boldsymbol{\mu}) \, \overline{P_{jl}(\mathbf{z}, \boldsymbol{\mu}, \mathbf{p}, \mathbf{q}_0)} \, \mathrm{d}\mathbf{z} \, \mathrm{d}\mathbf{q} \\
= &\frac{1}{(2\pi)^d} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu} \in \Lambda^*} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\mathbf{q} \cdot \mathbf{z}} \hat{N}(\mathbf{q}) \left[\sum_{m,n=1}^{2} \sigma_{mn}(t, \mathbf{x}, \mathbf{p}) Q_{mn}(\mathbf{z}, \boldsymbol{\mu}, \mathbf{p}) \right] \\
&\times \frac{1}{|\mathcal{C}|} \int_{\mathcal{C}} \mathrm{e}^{-\mathrm{i}(\mathbf{p} + \boldsymbol{\mu}) \cdot \mathbf{y}_2} \overline{\Psi_j(\mathbf{z} - \mathbf{y}_2, \mathbf{p})} \, \Psi_l(\mathbf{z}, \mathbf{p} + \mathbf{q}_0) \, \mathrm{d}\mathbf{y}_2 \, \mathrm{d}\mathbf{z} \, \mathrm{d}\mathbf{q} \\
= &\frac{1}{(2\pi)^d} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu} \in \Lambda^*} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\mathbf{q} \cdot \mathbf{z}} \hat{N}(\mathbf{q}) \\
&\times \left[\sum_{m,n=1}^{2} \sigma_{mn}(t, \mathbf{x}, \mathbf{p}) \frac{1}{|\mathcal{C}|} \int_{\mathcal{C}} \mathrm{e}^{\mathrm{i}(\mathbf{p} + \boldsymbol{\mu}) \cdot \mathbf{y}_1} \Psi_m(\mathbf{z} - \mathbf{y}_1, \mathbf{p}) \, \overline{\Psi_n(\mathbf{z}, \mathbf{p})} \, \mathrm{d}\mathbf{y}_1 \right] \\
&\times \frac{1}{|\mathcal{C}|} \int_{\mathcal{C}} \mathrm{e}^{-\mathrm{i}(\mathbf{p} + \boldsymbol{\mu}) \cdot \mathbf{y}_2} \overline{\Psi_j(\mathbf{z} - \mathbf{y}_2, \mathbf{p})} \, \Psi_l(\mathbf{z}, \mathbf{p} + \mathbf{q}_0) \, \mathrm{d}\mathbf{y}_2 \, \mathrm{d}\mathbf{z} \, \mathrm{d}\mathbf{q} \\
= &\frac{1}{(2\pi)^d} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu} \in \Lambda^*} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\mathbf{q} \cdot \mathbf{z}} \hat{N}(\mathbf{q}) \sum_{m,n=1}^{2} \sigma_{mn}(t, \mathbf{x}, \mathbf{p}) \frac{1}{|\mathcal{C}|^2} \int_{\mathcal{C}' \times \mathcal{C}'} \mathrm{e}^{\mathrm{i}(\mathbf{p} + \boldsymbol{\mu}) \cdot (\mathbf{y}_2 - \mathbf{y}_1)}
\end{aligned}
$$

$$
\begin{aligned}
&\times \Psi_m(\mathbf{y}_1,\mathbf{p})\,\overline{\Psi_j(\mathbf{y}_2,\mathbf{p})}\,\Psi_l(\mathbf{z},\mathbf{p}+\mathbf{q}_0)\,\overline{\Psi_n(\mathbf{z},\mathbf{p})}\,\mathrm{d}\mathbf{y}_1\,\mathrm{d}\mathbf{y}_2\,\mathrm{d}\mathbf{z}\,\mathrm{d}\mathbf{q}\\
&= \frac{1}{(2\pi)^d}\frac{1}{|\mathcal{B}|}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\hat{N}(\mathbf{q})\sum_{m,n=1}^{2}\sigma_{mn}(t,\mathbf{x},\mathbf{p})\Psi_l(\mathbf{z},\mathbf{p}+\mathbf{q}_0)\,\overline{\Psi_n(\mathbf{z},\mathbf{p})}\\
&\quad\times\frac{1}{|\mathcal{C}|}\int_{\mathcal{C}'\times\mathcal{C}'}\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot(\mathbf{y}_2-\mathbf{y}_1)}\sum_{\boldsymbol{\nu}\in\Lambda}\delta(\mathbf{y}_2-\mathbf{y}_1-\boldsymbol{\nu})\Psi_m(\mathbf{y}_1,\mathbf{p})\,\overline{\Psi_j(\mathbf{y}_2,\mathbf{p})}\,\mathrm{d}\mathbf{y}_1\,\mathrm{d}\mathbf{y}_2\,\mathrm{d}\mathbf{z}\,\mathrm{d}\mathbf{q}\\
&= \frac{1}{(2\pi)^d}\frac{1}{|\mathcal{B}|}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\hat{N}(\mathbf{q})\sum_{m,n=1}^{2}\sigma_{mn}(t,\mathbf{x},\mathbf{p})\Psi_l(\mathbf{z},\mathbf{p}+\mathbf{q}_0)\,\overline{\Psi_n(\mathbf{z},\mathbf{p})}\\
&\quad\times\frac{1}{|\mathcal{C}|}\int_{\mathcal{C}'}\sum_{\boldsymbol{\nu}\in\Lambda}\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\boldsymbol{\nu}}\Psi_m(\mathbf{y}_1,\mathbf{p})\,\overline{\Psi_j(\mathbf{y}_1+\boldsymbol{\nu},\mathbf{p})}\,\mathrm{d}\mathbf{y}_1\,\mathrm{d}\mathbf{z}\,\mathrm{d}\mathbf{q}\\
&= \frac{1}{(2\pi)^d}\frac{1}{|\mathcal{B}|}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\hat{N}(\mathbf{q})\sum_{m,n=1}^{2}\sigma_{mn}(t,\mathbf{x},\mathbf{p})\Psi_l(\mathbf{z},\mathbf{p}+\mathbf{q}_0)\,\overline{\Psi_n(\mathbf{z},\mathbf{p})}\\
&\quad\times\frac{1}{|\mathcal{C}|}\int_{\mathcal{C}'}\Psi_m(\mathbf{y}_1,\mathbf{p})\,\overline{\Psi_j(\mathbf{y}_1,\mathbf{p})}\,\mathrm{d}\mathbf{y}_1\,\mathrm{d}\mathbf{z}\,\mathrm{d}\mathbf{q}\\
&= \frac{1}{(2\pi)^d}\frac{1}{|\mathcal{B}|}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{z}}\hat{N}(\mathbf{q})\sum_{m,n=1}^{2}\sigma_{mn}(t,\mathbf{x},\mathbf{p})\delta_{mj}\Psi_l(\mathbf{z},\mathbf{p}+\mathbf{q}_0)\,\overline{\Psi_n(\mathbf{z},\mathbf{p})}\,\mathrm{d}\mathbf{z}\,\mathrm{d}\mathbf{q},
\end{aligned}
$$

where we apply the change of variables

$$\mathbf{y}_1\mapsto\mathbf{z}-\mathbf{y}_1,\quad \mathbf{y}_2\mapsto\mathbf{z}-\mathbf{y}_2$$

in the third inequality above, use the identity (A.3) in the fifth equality, as well as the periodicity of the Bloch eigenfunction $\overline{\Psi_j(\mathbf{y}_1+\boldsymbol{\nu},\mathbf{p})}=\mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\boldsymbol{\nu}}\overline{\Psi_j(\mathbf{y}_1,\mathbf{p})}$ in the second to the last equality.

Appendix C. Explicit form of the random system away from band crossings. We now show how the system (4.16) reduces to [3, eq. (3.15)] whenever $\mathbf{p}$ is away from band crossings. Recalling the discussion in section 3.2, we assume that the bands touch at finitely many crossing points $\mathbf{p}_*$ with a structure given by (3.21) for some integers $r>0$. In this case, assuming $|\mathbf{p}-\mathbf{p}_*|\gg\varepsilon^{1/r}$ as $\varepsilon\downarrow 0$, we can replace the terms in (4.16) after taking the weak limit as $\varepsilon\downarrow 0$:

$$
\begin{aligned}
&\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}[E_l(\mathbf{p})-E_n(\mathbf{p})]t}\to\delta(E_l(\mathbf{p})-E_n(\mathbf{p}))\to\delta_{ln}\,,\\
&\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}[E_m(\mathbf{q})-E_{m'}(\mathbf{q})+E_l(\mathbf{p})-E_j(\mathbf{p})]t}\to\delta(E_m(\mathbf{q})-E_{m'}(\mathbf{q})+E_l(\mathbf{p})-E_j(\mathbf{p}))\,,\\
&\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}[E_{m'}(\mathbf{p})-E_j(\mathbf{p})]t}\to\delta(E_{m'}(\mathbf{p})-E_j(\mathbf{p}))\to\delta_{m'j}
\end{aligned}
\tag{C.1}
$$

and therefore we have

$$
\begin{aligned}
&\partial_t\widetilde{\sigma}_{jl}(t,\mathbf{x},\mathbf{p})+\nabla_{\mathbf{x}}\widetilde{\sigma}_{jl}(t,\mathbf{x},\mathbf{p})\cdot\langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_l,\Psi_l\rangle_{\mathcal{C}}\\
&\quad=\sum_{m=1}^{2}\frac{1}{(2\pi)^{d-1}}\frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{\mu}\in\Lambda^*}\int_{\mathcal{B}}\hat{R}(\mathbf{p}-\mathbf{q}+\boldsymbol{\mu})\delta(E_l(\mathbf{p})-E_m(\mathbf{q}))\overline{A_{jm}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})}\\
&\qquad\times\Bigg[\sum_{m'=1}^{2}\delta(E_m(\mathbf{q})-E_{m'}(\mathbf{q})+E_l(\mathbf{p})-E_j(\mathbf{p}))\widetilde{\sigma}_{mm'}(\mathbf{q})A_{lm'}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})\\
&\qquad-\widetilde{\sigma}_{jl}(\mathbf{p})A_{jm}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})\Bigg]\,\mathrm{d}\mathbf{q}.
\end{aligned}
\tag{C.2}
$$

(C.2) then provides the explicit dynamics for the diagonal terms $\widetilde{\sigma}_{jl}, j = l$ and off-diagonal terms $\widetilde{\sigma}_{jl}, j \neq l$, respectively:

- When $j = l$, $\delta(E_m(\mathbf{q}) - E_{m'}(\mathbf{q}) + E_l(\mathbf{p}) - E_j(\mathbf{p}))$ in (C.2) simplifies to

$$\delta(E_m(\mathbf{q}) - E_{m'}(\mathbf{q}) + E_l(\mathbf{p}) - E_j(\mathbf{p})) \to \delta_{mm'}$$

so that we have, after replacing $\langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_j, \Psi_j\rangle_{\mathcal{C}}$ by $\nabla_{\mathbf{p}} E_j(\mathbf{p})$,

(C.3)
$$\partial_t \widetilde{\sigma}_{jj}(t,\mathbf{x},\mathbf{p}) + \nabla_{\mathbf{x}} \widetilde{\sigma}_{jj}(t,\mathbf{x},\mathbf{p}) \cdot \nabla_{\mathbf{p}} E_j(\mathbf{p}) \\ = \sum_{m=1}^{2} \frac{1}{(2\pi)^{d-1}} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu}\in\Lambda^*} \int_{\mathcal{B}} \hat{R}(\mathbf{p}-\mathbf{q}+\boldsymbol{\mu})\delta(E_l(\mathbf{p})-E_m(\mathbf{q}))|A_{jm}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})|^2 \\ \times \Big[\widetilde{\sigma}_{mm}(\mathbf{q}) - \widetilde{\sigma}_{jj}(\mathbf{p})\Big]\,\mathrm{d}\mathbf{q},$$

which is exactly [3, eq. (3.15)].

- When $j \neq l$, a case-by-case analysis (listing all cases for $j, l, m, m' \in \{1, 2\}$) shows that we can replace $\delta(E_m(\mathbf{q}) - E_{m'}(\mathbf{q}) + E_l(\mathbf{p}) - E_j(\mathbf{p}))$ by

$$\delta(E_m(\mathbf{q})-E_{m'}(\mathbf{q})+E_l(\mathbf{p})-E_j(\mathbf{p})) \to \delta_{jm}\delta_{lm'}\delta(E_j(\mathbf{q})-E_l(\mathbf{q})+E_l(\mathbf{p})-E_j(\mathbf{p})),$$

so that (C.2) becomes

(C.4)
$$\partial_t \widetilde{\sigma}_{jl}(t,\mathbf{x},\mathbf{p}) + \nabla_{\mathbf{x}} \widetilde{\sigma}_{jl}(t,\mathbf{x},\mathbf{p}) \cdot \langle(-\mathrm{i}\nabla_{\mathbf{z}})\Psi_l, \Psi_l\rangle_{\mathcal{C}} \\ = \sum_{m=1}^{2} \frac{1}{(2\pi)^{d-1}} \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{\mu}\in\Lambda^*} \int_{\mathcal{B}} \hat{R}(\mathbf{p}-\mathbf{q}+\boldsymbol{\mu})\delta(E_l(\mathbf{p})-E_m(\mathbf{q}))\overline{A_{jm}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})} \\ \times \Big[\delta(E_j(\mathbf{q}) - E_l(\mathbf{q}) + E_l(\mathbf{p}) - E_j(\mathbf{p}))\widetilde{\sigma}_{jl}(\mathbf{q})A_{ll}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu}) \\ - \widetilde{\sigma}_{jl}(\mathbf{p})A_{jm}(\mathbf{p},\mathbf{q}-\boldsymbol{\mu})\Big]\,\mathrm{d}\mathbf{q}.$$

In particular, each $\widetilde{\sigma}_{jl}$ evolves under a closed equation, ensuring that if the off-diagonal terms $\widetilde{\sigma}, j \neq l$ are initially zero, they remain zero for all t. This confirms that the off-diagonal σ terms can be neglected away from band crossings as expected.

Acknowledgments. We acknowledge helpful discussions with Guillaume Bal, John Schotland, and Michael Hott. We also thank the anonymous reviewers for their valuable comments and suggestions, which significantly helped improve the quality of the paper.

REFERENCES

[1] G. Allaire, A. Arnold, P. Degond, and T. Y. Hou, *Quantum Transport*, Springer, Berlin, 2008.

[2] G. Bal, P. Cazeaux, D. Massatt, and S. Quinn, *Mathematical models of topologically protected transport in twisted bilayer graphene*, Multiscale Model. Simul., 21 (2023), pp. 1081–1121, https://doi.org/10.1137/22M1505542.

[3] G. Bal, A. Fannjiang, G. Papanicolaou, and L. Ryzhik, *Radiative transport in a periodic structure*, J. Stat. Phys., 95 (1999), pp. 479–494, https://doi.org/10.1023/A:1004598015978.

[4] G. Bal, Y. Gu, and O. Pinaud, *Radiative transport limit of Dirac equations with random electromagnetic field*, Comm. Partial Differential Equations, 43 (2018), pp. 699–732, https://doi.org/10.1080/03605302.2018.1472105.

[5] G. Bal, G. Papanicolaou, and L. Ryzhik, *Radiative transport limit for the random Schrödinger equation*, Nonlinearity, 15 (2002), pp. 513–529, https://doi.org/10.1088/0951-7715/15/2/315.

[6] P. Bechouche, N. J. Mauser, and F. Poupaud, *Semiclassical limit for the Schrödinger-Poisson equation in a crystal*, Comm. Pure Appl. Math., 54 (2001), pp. 851–890, https://doi.org/10.1002/cpa.3004.

[7] S. Becker, S. Quinn, Z. Tao, A. Watson, and M. Yang, *Dirac cones and magic angles in the Bistritzer–Macdonald TBG Hamiltonian*, preprint, https://arxiv.org/abs/2407.06316, 2024.

[8] A. Bensoussan, J.-L. Lions, and G. Papanicolaou, *Asymptotic Analysis for Periodic Structures*, Stud. Math. Appl. 5, North-Holland, Amsterdam, 1978.

[9] G. Berkolaiko and A. Comech, *Symmetry and Dirac points in graphene spectrum*, J. Spectr. Theory, 8 (2018), pp. 1099–1147, https://doi.org/10.4171/jst/223.

[10] P. L. Bhatnagar, E. P. Gross, and M. Krook, *A model for collision processes in gases*, Phys. Rev. (2), 94 (1954), pp. 511–514, https://doi.org/10.1103/PhysRev.94.511.

[11] R. Bistritzer and A. H. MacDonald, *Moiré bands in twisted double-layer graphene*, Proc. Natl. Acad. Sci. USA, 108 (2011), pp. 12233–12237, https://doi.org/10.1073/pnas.1108174108.

[12] Y. Cao, V. Fatemi, A. Demir, S. Fang, S. L. Tomarken, J. Y. Luo, J. D. Sanchez-Yamagishi, K. Watanabe, T. Taniguchi, E. Kaxiras, R. C. Ashoori, and P. Jarillo-Herrero, *Correlated insulator behaviour at half-filling in magic-angle graphene superlattices*, Nature, 556 (2018), pp. 80–84, https://doi.org/10.1038/nature26154.

[13] Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E. Kaxiras, and P. Jarillo-Herrero, *Unconventional superconductivity in magic-angle graphene superlattices*, Nature, 556 (2018), pp. 43–50, https://doi.org/10.1038/nature26160.

[14] L. Chai, S. Jin, and Q. Li, *Semi-classical models for the Schrödinger equation with periodic potentials and band crossings*, Kinet. Relat. Models, 6 (2013), pp. 505–532, https://doi.org/10.3934/krm.2013.6.505.

[15] J. C. T. David and S. Sholl, *A generalized surface hopping method*, J. Chem. Phys., 109 (1998), pp. 7702–7710, https://doi.org/10.1063/1.477416.

[16] K. Drukker, *Basics of surface hopping in mixed quantum/classical simulations*, J. Comput. Phys., 153 (1999), pp. 225–272, https://doi.org/10.1006/jcph.1999.6287.

[17] L. Erdős and H.-T. Yau, *Linear Boltzmann equation as the weak coupling limit of a random Schrödinger equation*, Comm. Pure Appl. Math., 53 (2000), pp. 667–735, https://doi.org/10.1002/(SICI)1097-0312(200006)53:6⟨667::AID-CPA1⟩3.0.CO;2-5.

[18] A. Fannjiang, G. Papanicolaou, and S. Jin, *High frequency behavior of the focusing nonlinear Schrödinger equation with random inhomogeneities*, SIAM J. Appl. Math., 63 (2003), pp. 1328–1358, https://doi.org/10.1137/S003613999935559X.

[19] C. L. Fefferman and M. I. Weinstein, *Honeycomb lattice potentials and Dirac points*, J. Amer. Math. Soc., 25 (2012), pp. 1169–1220, https://doi.org/10.1090/S0894-0347-2012-00745-0.

[20] C. L. Fefferman and M. I. Weinstein, *Wave packets in honeycomb structures and two-dimensional Dirac equations*, Comm. Math. Phys., 326 (2014), pp. 251–286, https://doi.org/10.1007/s00220-013-1847-2.

[21] C. Fermanian-Kammerer, *Semiclassical analysis of generic codimension* 3 *crossings*, Int. Math. Res. Not. IMRN, 2004 (2004), pp. 2391–2435, https://doi.org/10.1155/S1073792804133175.

[22] C. Fermanian-Kammerer, P. Gérard, and C. Lasser, *Wigner measure propagation and conical singularity for general initial data*, Arch. Ration. Mech. Anal., 209 (2013), pp. 209–236, https://doi.org/10.1007/s00205-013-0622-z.

[23] C. Fermanian-Kammerer and C. Lasser, *Wigner measures and codimension two crossings*, J. Math. Phys., 44 (2003), pp. 507–527, https://doi.org/10.1063/1.1527221.

[24] P. Gérard, *Mesures semi-classiques et ondes de Bloch*, in *Séminaire sur les Équations aux Dérivées Partielles,* 1990-1991, *École Polytech*, Palaiseau, Paris, 1991, pp. Exp. No. XVI, 19.

[25] P. Gérard and E. Leichtnam, *Ergodic properties of eigenfunctions for the Dirichlet problem*, Duke Math. J., 71 (1993), pp. 559–607, https://doi.org/10.1215/S0012-7094-93-07122-0.

[26] P. Gérard, P. A. Markowich, N. J. Mauser, and F. Poupaud, *Homogenization limits and Wigner transforms*, Comm. Pure Appl. Math., 50 (1997), pp. 323–379, https://onlinelibrary.wiley.com/doi/abs/10.1002/%28SICI%291097-0312%28199704%2950%3A4%3C323%3A%3AAID-CPA4%3E3.0.CO%3B2-C.

[27] G. A. Hagedorn, *Molecular propagation through electron energy level crossings*, Memoirs of the American Mathematical Society, Vol. 111, American Mathematical Society, Providence, RI, 1994, https://doi.org/10.1090/memo/0536.

[28] T. G. Ho, L. J. Landau, and A. J. Wilkins, *On the weak coupling limit for a Fermi gas in a random potential*, Rev. Math. Phys., 5 (1993), pp. 209–298, https://doi.org/10.1142/S0129055X93000061.

[29] S. Jin and Z. P. Xin, *The relaxation schemes for systems of conservation laws in arbitrary space dimensions*, Comm. Pure Appl. Math., 48 (1995), pp. 235–276, https://doi.org/10.1002/cpa.3160480303.

[30] R. K. P. John and C. Tully, *Trajectory surface hopping approach to nonadiabatic molecular collisions: The reaction of h+ with d2*, J. Chem. Phys., 55 (1971), pp. 562–572, https://doi.org/10.1063/1.1675788.

[31] L. D. Landau, *Zur theorie der energieübertragung,* II, Phys. Sov. Union, 2 (1932), pp. 46–51.

[32] C. Lasser, T. Swart, and S. Teufel, *Construction and validation of a rigorous surface hopping algorithm for conical crossings*, Commun. Math. Sci., 5 (2007), pp. 789–814, https://doi.org/10.4310/CMS.2007.v5.n4.a3.

[33] C. Lasser and S. Teufel, *Propagation through conical crossings: An asymptotic semigroup*, Comm. Pure Appl. Math., 58 (2005), pp. 1188–1230, https://doi.org/10.1002/cpa.20087.

[34] P.-L. Lions and T. Paul, *Sur les mesures de Wigner*, Rev. Mat. Iberoam., 9 (1993), pp. 553–618, https://doi.org/10.4171/rmi/143.

[35] P. A. Markowich and N. J. Mauser, *The classical limit of a self-consistent quantum-Vlasov equation in 3d*, Math. Models Methods Appl. Sci., 03 (1993), pp. 109–124, https://doi.org/10.1142/S0218202593000072.

[36] P. A. Markowich, N. J. Mauser, and F. Poupaud, *A Wigner-function approach to (semi)classical limits: Electrons in a periodic potential*, J. Math. Phys., 35 (1994), pp. 1066–1094, https://doi.org/10.1063/1.530629.

[37] A. H. C. Neto, N. M. R. P. F. Guinea, K. S. Novoselov, and A. K. Geim, *The electronic properties of graphene*, Rev. Modern Phys., 81 (2009), pp. 109–162, https://doi.org/10.1103/RevModPhys.81.109.

[38] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov, *Two-dimensional gas of massless Dirac fermions in graphene*, Nature, 438 (2005), pp. 197–200, https://doi.org/10.1038/nature04233.

[39] F. Odeh and J. B. Keller, *Partial differential equations with periodic coefficients and Bloch waves in crystals*, J. Math. Phys., 5 (1964), pp. 1499–1504, https://doi.org/10.1063/1.1931182.

[40] L. Ryzhik, G. Papanicolaou, and J. B. Keller, *Transport equations for elastic and other waves in random media*, Wave Motion, 24 (1996), pp. 327–370, https://doi.org/10.1016/S0165-2125(96)00021-2.

[41] L. Ryzhik, G. Papanicolaou, and J. B. Keller, *Transport equations for waves in a half space*, Comm. Partial Differential Equations, 22 (1997), pp. 1869–1910, https://doi.org/10.1080/03605309708821324.

[42] H. Spohn, *Derivation of the transport equation for electrons moving through random impurities*, J. Stat. Phys., 17 (1977), pp. 385–412, https://doi.org/10.1007/BF01014347.

[43] D. Vanderbilt, *Berry Phases in Electronic Structure Theory: Electric Polarization, Orbital Magnetization and Topological Insulators*, Cambridge University Press, Cambridge, 2018.

[44] A. Watson and M. I. Weinstein, *Wavepackets in inhomogeneous periodic media: Propagation through a one-dimensional band crossing*, Comm. Math. Phys., 363 (2018), pp. 655–698, https://doi.org/10.1007/s00220-018-3213-x.

[45] E. Wigner, *On the quantum correction for thermodynamic equilibrium*, Phys. Rev. (2), 40 (1932), pp. 749–759, https://doi.org/10.1103/PhysRev.40.749.

[46] C. H. Wilcox, *Theory of Bloch waves*, J. Anal. Math., 33 (1978), pp. 146–167, https://doi.org/10.1007/BF02790171.

[47] C. Zener, *Non-adiabatic crossing of energy levels*, Proc. Roy. Soc. Lond. Ser. A, 137 (1932), pp. 696–702, https://doi.org/10.1098/rspa.1932.0165.