RIGOROUS DERIVATION OF NONLINEAR DIRAC EQUATIONS FOR WAVE PROPAGATION IN HONEYCOMB STRUCTURES

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ABSTRACT. We consider a nonlinear Schrödinger equation in two spatial dimensions subject to a periodic honeycomb lattice potential. Using a multiscale expansion together with rigorous error estimates, we derive an effective model of nonlinear Dirac type. The latter describes the propagation of slowly modulated, weakly nonlinear waves spectrally localized near a Dirac point.

1. INTRODUCTION

Two-dimensional honeycomb lattice structures have attracted considerable interest in both physics and applied mathematics due to their unusual transport properties. This has been particularly stimulated by the recent fabrication of *graphene*, a mono-crystalline graphitic film in which electrons behave like two-dimensional *Dirac fermions* without mass, cf. [9] for a recent review. Honeycomb structures also appear in nonlinear optics, modeling laser beam propagation in certain types of photonic crystals, see, e.g., [3, 21] for more details. In both situations, the starting point is a two-dimensional Schrödinger operator

$$(1.1) \qquad H = -\Delta + V_{\mathrm{per}}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^2,$$

where $V_{\mathrm{per}} \in C^\infty(\mathbb{R}^2; \mathbb{R})$, denotes a smooth potential which is periodic with respect to a honeycomb lattice Λ with fundamental cell $Y \subset \Lambda$ (see Section 2 below for more details). C. L. Fefferman and M. I. Weinstein in their seminal paper [16] proved that the associated quasi-particle dispersion relation generically exhibits conical singularities at the points of degeneracy, the so-called *Dirac points*. In turn, this yields effective equations of (massless) Dirac type for wave packets spectrally localized around these singularities, see [1, 17, 18].

To be more precise, let us recall that, by basic *Bloch-Floquet theory*, the spectrum $\sigma(H) \subset \mathbb{R}$ is given by a union of spectral bands, which can be obtained through the following $\mathbf{k}$−pseudo periodic boundary value problem [30]:

$$(1.2) \qquad \begin{cases} H\Phi(\mathbf{y}; \mathbf{k}) = \mu(\mathbf{k})\Phi(\mathbf{y}; \mathbf{k}), \ \mathbf{y} \in Y, \\ \Phi(\mathbf{y} + \mathbf{v}; \mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{v}}\Phi(\mathbf{y}; \mathbf{k}), \ \mathbf{v} \in \Lambda, \end{cases}$$

where $\mathbf{k} \in Y^*$ denotes the wave-vector (or, quasi-momentum) varying within the Brioullin zone, i.e., the fundamental cell of the dual lattice Λ^*. This yields a countable sequence of real-valued eigenvalues which are ordered, including multiplicity, such that

$$\mu_0(\mathbf{k}) \leqslant \mu_1(\mathbf{k}) \leqslant \mu_2(\mathbf{k}) \leqslant ...,$$

They describe the effective dispersion relation within the periodic structure. The corresponding pseudo-periodic eigenfunctions $\Phi_m(\,\cdot\,; \mathbf{k})$, are known as *Bloch waves*.

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They form, for every fixed $\mathbf{k} \in Y^*$ a complete orthonormal basis on $L^2(Y)$. This consequently allows one to write the linear time-evolution associated to (2.2) as

$$\Psi(t, \mathbf{x}) = e^{-iHt}\Psi_0(\mathbf{x}) = \sum_{m \geqslant 1} \int_{Y^*} e^{-i\mu_m(\mathbf{k})t}\langle \Phi_m(\,\cdot\,; \mathbf{k}), \Psi_0 \rangle_{L^2(\mathbb{R}^2)} \Phi_m(\mathbf{x}; \mathbf{k})\, d\mathbf{k},$$

for any initial data $\Psi_0 \in L^2(\mathbb{R}^2)$.

In the following, let the index $m \geqslant 1$ be fixed (to be suppressed henceforth) and assume that at $\mathbf{k} = \mathbf{K}_*$, the m-th band $\mu_* \equiv \mu(\mathbf{K}_*)$, has a Dirac point, such that

$$\text{Nullspace}(H - \mu_*) = \text{span}\left\{\Phi_1(\mathbf{x}), \Phi_2(\mathbf{x})\right\},$$

cf. Section 2 below for a precise definition. Furthermore, let $0 < \varepsilon \ll 1$ be a small (dimensionless) parameter, and assume that initially $\Psi_0 = \Psi_0^\varepsilon$ is a wave packet, spectrally concentrated around this Dirac point, i.e.,

$$\Psi_0^\varepsilon(\mathbf{x}) = \varepsilon\alpha_{0,1}(\varepsilon\mathbf{x})\Phi_1(\mathbf{x}) + \varepsilon\alpha_{0,2}(\varepsilon\mathbf{x})\Phi_2(\mathbf{x})$$

where $\alpha_{0,1}, \alpha_{0,2} \in \mathcal{S}(\mathbb{R}^2; \mathbb{C})$ are some slowly varying and rapidly decaying amplitudes. The overall factor ε is thereby introduced to ensure that $\|\Psi_0\|_{L^2} = 1$. It is proved in [18] that the corresponding solution $\Psi^\varepsilon(t, \cdot)$ of the linear Schrödinger equation satisfies,

$$\Psi^\varepsilon(t, \mathbf{x}) \underset{\varepsilon \to 0}{\sim} \varepsilon e^{-i\mu_* t}\Big(\alpha_1(\varepsilon t, \varepsilon\mathbf{x})\Phi_1(\mathbf{x}) + \alpha_2(\varepsilon t, \varepsilon\mathbf{x})\Phi_2(\mathbf{x})\Big),$$

provided $\alpha_{1,2}$ satisfy the following massless Dirac system:

(1.3) $$\begin{cases} \partial_t\alpha_1 + \overline{\lambda}_\#\big(\partial_{x_1} + i\partial_{x_2}\big)\alpha_2 = 0, & \alpha_{1|t=0} = \alpha_{0,1}, \\ \partial_t\alpha_2 + \lambda_\#\big(\partial_{x_1} - i\partial_{x_2}\big)\alpha_1 = 0, & \alpha_{2|t=0} = \alpha_{0,2}, \end{cases}$$

where $0 \neq \lambda_\# \in \mathbb{C}$ is some constant depending on V_{per}. This approximation is shown to hold up to small errors in $H^s(\mathbb{R}^2)$, over time-intervals of order $T \sim \mathcal{O}(\varepsilon^{-2+\delta})$, for $\delta > 0$. The Dirac system (1.3) consequently describes the dynamics of the slowly varying amplitudes on large time scales. Of course, since the problem is linear, solutions of any size (w.r.t. ε) will satisfy the same asymptotic behavior.

In the present work, we aim to generalize this type of result to the case of *weakly nonlinear* wave packets. Formally, this problem was described in [17], but without providing any rigorous error estimates. Similarly, in [1, 2] the authors derive several nonlinear Dirac type models by a formal multi-scale expansions in the case of *deformed* and *shallow* honeycomb lattice structures, respectively. In the latter case, the size of the lattice potential serves as the small parameter in the expansion. In contrast to that, we shall not assume that the periodic potential V_{per} is small, but rather keep it of a fixed size of order $\mathcal{O}(1)$, i.e., independent of ε, in $L^\infty(\mathbb{R}^2)$. However, as always in nonlinear problems, the size of the solution becomes important (depending on the power of the nonlinearity). To this end, we find it more convenient to put ourselves in a *macroscopic reference frame*, which means that we re-scale

$$t \mapsto \tilde{t} = \varepsilon t, \quad x \mapsto \tilde{\mathbf{x}} = \varepsilon\mathbf{x}, \quad \tilde{\Psi}^\varepsilon(\tilde{t}, \tilde{\mathbf{x}}) = \varepsilon\Psi^\varepsilon(\varepsilon t, \varepsilon\mathbf{x}),$$

with $\|\Psi_0^\varepsilon(t, \cdot)\|_{L^2} = 1$. We consequently consider the following, *semi-classically scaled* nonlinear Schrödinger equation (NLS), after having dropped all " ~ " again:

(1.4) $$i\varepsilon\partial_t\Psi^\varepsilon = -\varepsilon^2\Delta\Psi^\varepsilon + V_{\text{per}}\Big(\frac{\mathbf{x}}{\varepsilon}\Big)\Psi^\varepsilon + \kappa^\varepsilon|\Psi^\varepsilon|^2\Psi^\varepsilon, \quad \Psi_{|t=0}^\varepsilon = \Psi_0^\varepsilon(\mathbf{x}).$$

Notice that in this reference frame the honeycomb lattice potential becomes *highly oscillatory*. We restrict ourselves to the case of NLS with cubic nonlinearities, since they are the most important ones within the context of nonlinear optics (a generalization to other power law nonlinearities is straightforward). However, we shall also remark on the case of *Hartree nonlinearities* in Section 6 below, as they are

more natural in the description of the mean-field dynamics of electrons in graphene [21, 23]. The nonlinear coupling constant $\kappa^\varepsilon \in \mathbb{R}$, is assumed to be of the form

$$\kappa^\varepsilon = \varepsilon\kappa, \quad \text{with } \kappa = \pm 1.$$

As will become clear, this size is *critical* with respect to our asymptotic expansion, in the sense that the associated modulating amplitudes $\alpha_{1,2}$ will satisfy a nonlinear analog of (1.3). For smaller κ^ε, no nonlinear effects are present in leading order, as $\varepsilon \to 0$, whereas for κ^ε larger than $\mathcal{O}(\varepsilon)$, we do not expect the Dirac model to be valid any longer. Alternatively, this can be reformulated as saying that we consider asymptotically small solutions of critical size $\mathcal{O}(\sqrt{\varepsilon})$ in L^∞ to (1.4) but with fixed coupling strength $\kappa = \mathcal{O}(1)$. The advantage of our scaling is that it yields an asymptotic description for solutions of order $\mathcal{O}(1)$ in L^∞ on macroscopic space-time scales, in contrast to the setting of [1, 17], in which the size of the solution varies as $\varepsilon \to 0$. Another advantage is that this scaling puts us firmly in the regime of weakly nonlinear, semi-classical NLS with highly oscillatory periodic potentials, which have been extensively studied in, e.g., [5, 6, 7, 8, 19], albeit not for the case of honeycomb lattices. From the mathematical point of view, the present work will follow the ideas presented in [19] and adapt them to the current situation.

Our main result, described in more detail in Section 5, rigorously shows that solutions to (1.4) with initial data Ψ_0^ε spectrally localized around a Dirac point, can be approximated via

$$(1.5) \qquad \Psi^\varepsilon(t, \mathbf{x}) \underset{\varepsilon \to 0}{\sim} e^{-i\mu_* t/\varepsilon} \left(\alpha_1(t, \mathbf{x}) \Phi_1\left(\frac{\mathbf{x}}{\varepsilon}\right) + \alpha_2(t, \mathbf{x}) \Phi_2\left(\frac{\mathbf{x}}{\varepsilon}\right) \right) + \mathcal{O}(\varepsilon),$$

where the amplitudes $\alpha_{1,2}$ solve the following nonlinear Dirac system

$$(1.6) \qquad \begin{cases} \partial_t \alpha_1 + \overline{\lambda}_{\#}\left(\partial_{x_1} + i\partial_{x_2}\right)\alpha_2 = -i\kappa\left(b_1|\alpha_1|^2 + 2b_2|\alpha_2|^2\right)\alpha_1, \\ \partial_t \alpha_2 + \lambda_{\#}\left(\partial_{x_1} - i\partial_{x_2}\right)\alpha_1 = -i\kappa\left(b_1|\alpha_2|^2 + 2b_2|\alpha_1|^2\right)\alpha_2, \end{cases}$$

subject to initial data $\alpha_{0,1}(\mathbf{x})$, $\alpha_{0,2}(\mathbf{x})$, respectively, and with coefficients $b_{1,2} > 0$ given by

$$b_1 = \int_Y |\Phi_1(\mathbf{y})|^4 \, d\mathbf{y} = \int_Y |\Phi_2(\mathbf{y})|^4 \, d\mathbf{y}, \quad b_2 = \int_Y |\Phi_1(\mathbf{y})|^2 |\Phi_2(\mathbf{y})|^2 \, d\mathbf{y}.$$

The nonlinear Dirac system (1.6) has been formally derived in [17] and plays the same role as the coupled mode equations derived in [19], or the semi-classical transport equations derived in [5, 8]. This becomes even more apparent when we recall that the Bloch waves $\Phi_{1,2}$ can be written as

$$\Phi_{1,2}\left(\frac{\mathbf{x}}{\varepsilon}\right) = \chi_{1,2}\left(\frac{\mathbf{x}}{\varepsilon}\right) e^{i\mathbf{K}_* \cdot \mathbf{x}/\varepsilon},$$

where now $\chi_{1,2}(\cdot)$ is purely Λ-periodic. This shows that (1.5) is of the form of a two-scale Wentzel-Kramers-Brillouin (WKB) ansatz, first introduced in [5], involving a highly oscillatory phase function

$$S(t, x) = \mathbf{K}_* \cdot \mathbf{x} - \mu_* t.$$

The latter is seen to be the unique, global in time, smooth solution (i.e., no caustics) of the *semi-classical Hamilton-Jacobi equation*

$$\partial_t S + \mu(\nabla S) = 0, \quad S(0, \mathbf{x}) = \mathbf{K}_* \cdot \mathbf{x}.$$

The fact that the phase function S does not suffer from caustics, allows us to prove that our approximation (1.5) holds for (finite) time-intervals of order $\mathcal{O}(1)$, bounded by the existence time of (1.6). In contrast to that, it is known from earlier results, cf. [5, 8], that caustics within S lead to the breakdown of a single-phase WKB

approximation. Also note that the group velocity $\nabla S = \mathbf{K}_*$ being constant allows us to localize around Dirac points.

In terms of the unscaled variables used in [17, 18], our approximation result is seen to hold on times of order $\mathcal{O}(\varepsilon^{-1})$, which is considerably shorter than the time-scale $O(\varepsilon^{-2+\delta})$ obtained in [17]. This drawback, however, is expected due to the influence of our nonlinear perturbation and consistent with earlier results for linear semi-classical Schrödinger equations with periodic potentials and additional, slowly varying non-periodic perturbations $U = U(t, x)$, see, e.g., [5]. In the case of the latter, one also expects the appearance of purely geometric effects, such as the celebrated Berry phase term (cf. [6, 8]). It would certainly be interesting to understand the corresponding Dirac-type dynamics already on the linear level, when such geometric effects are present (but this is beyond the scope of the current work). We finally note that other examples of coupled mode equations have been derived in, e.g., [11, 12, 20, 26, 27]. In these models, however, the resulting mode equations are of transport type, and any coupling between the amplitudes stems purely from the nonlinearity, in contrast to the Dirac model. We finally remark that discrete mode equations, valid in the tight binding regime, have recently been studied in [2, 15].

This paper is now organized as follows: In Section 2 we recall some basic properties of honeycomb lattice structures and the associated lattice potentials. Then, we shall perform a formal multi-scale expansion in Section 3, for which we will set up a rigorous framework in Section 4. As a last step, we shall prove in Section 5 that the approximate solutions thereby obtained is stable under the nonlinear time evolution of the NLS. Finally, we shall briefly discuss the case of Hartree nonlinearities in Section 6.

2. Mathematical preliminaries

2.1. Honeycomb lattice potentials.

We start by recalling the basic geometry of triangular lattices arising naturally in the connection to honeycomb structures. Let $\Lambda = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2$, spanned by

$$\mathbf{v}_1 = a \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, \quad \mathbf{v}_2 = a \begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{1}{2} \end{pmatrix}, \quad a > 0.$$

Then, the honeycomb structure H is the union of two sub-lattices $\Lambda_{\mathbf{A}} = \mathbf{A} + \Lambda$ and $\Lambda_{\mathbf{B}} = \mathbf{B} + \Lambda$, cf. [16, 17]. The corresponding dual lattice $\Lambda^* = \mathbb{Z}\mathbf{k}_1 \oplus \mathbb{Z}\mathbf{k}_2$ is spanned by the dual basis vectors

$$\mathbf{k}_1 = q \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}, \quad \mathbf{k}_2 = q \begin{pmatrix} \frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix}, \quad q \equiv \frac{4\pi}{a\sqrt{3}},$$

such that $\mathbf{v}_j \cdot \mathbf{k}_j = 2\pi$. The fundamental period cell is denoted by

$$Y = \{\theta_1 v_1 + \theta_2 v_2 : 0 \leqslant \theta_j \leqslant 1, j = 1, 2\}.$$

In the following, we shall denote $L_{\text{per}}^2 \equiv L^2(\mathbb{R}^2/\Lambda)$ and likewise for other function spaces. An element $f \in L_{\text{per}}^2$ is called Λ-periodic, since it satisfies

$$f(\mathbf{y} + \mathbf{v}) = f(\mathbf{y}), \quad \text{for all } \mathbf{y} \in \mathbb{R}^2 \text{ and } \mathbf{v} \in \Lambda.$$

On the other hand, we shall denote $f \in L_{\mathbf{k}}^2$ and call it $\mathbf{k}-$pseudo periodic, if

$$f(\mathbf{y} + \mathbf{v}) = f(\mathbf{y})e^{i\mathbf{k}\cdot\mathbf{v}} \quad \text{for all } \mathbf{y} \in \mathbb{R}^2 \text{ and } \mathbf{v} \in \Lambda.$$

The Brillouin zone, Y^*, is a choice of fundamental unit cell in the dual period lattice which we choose to be a regular hexagon centered at the origin. Due to

symmetry, the vertices of Y^* fall into two equivalence classes of points, $\mathbf{K} \equiv \frac{1}{3}(\mathbf{k}_1 + \mathbf{k}_2)$ and $\mathbf{K}' \equiv -\mathbf{K} = \frac{1}{3}(\mathbf{k}_2 - \mathbf{k}_1)$. The other vertices are generated by the action of $2\pi/3$ rotation matrix, R given by

$$R = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix},$$

so that

$$R\mathbf{K} = \mathbf{K} + \mathbf{k}_2, \quad R^2\mathbf{K} = \mathbf{K} - \mathbf{k}_1.$$
$$R\mathbf{K}' = \mathbf{K}' - \mathbf{k}_2, \quad R^2\mathbf{K}' = \mathbf{K}' + \mathbf{k}_1.$$

Let $\mathbf{K}_*$ be a vertex of $\mathbf{K}$ or $\mathbf{K}'$ type. For any function $f \in L^2_{\mathbf{K}_*}$, we introduce the unitary operator

(2.1) $$\mathcal{R} : f \mapsto \mathcal{R}[f] = f(R^*\mathbf{y}) = f(R^{-1}\mathbf{y}).$$

One checks that $\mathcal{R}$ has eigenvalues $1, \tau, \bar{\tau}$, where $\tau = e^{2\pi i/3}$. This consequently yields the following pairwise orthogonal subspaces

$$L^2_{\mathbf{K}_*,1} \equiv \{f \in L^2_{\mathbf{K}_*} : \mathcal{R}[f] = f\}$$
$$L^2_{\mathbf{K}_*,\tau} \equiv \{f \in L^2_{\mathbf{K}_*} : \mathcal{R}[f] = \tau f\}$$
$$L^2_{\mathbf{K}_*,\bar{\tau}} \equiv \{f \in L^2_{\mathbf{K}_*} : \mathcal{R}[f] = \bar{\tau} f\},$$

to be used later on.

In [16], the following class of potentials, which yields such honeycomb lattice structures, has been introduced:

Definition 2.1. Let $V \in C^\infty(\mathbb{R}^2; \mathbb{R})$. Then V is called a **honeycomb lattice potential** if there exists an $\mathbf{y}_0 \in \mathbb{R}^2$ such that $\tilde{V} = V(\mathbf{y} - \mathbf{y}_0)$ has the following properties :

(1) $\tilde{V}$ is Λ-periodic.
(2) $\tilde{V}$ is inversion symmetric, i.e., $\tilde{V}(-\mathbf{y}) = \tilde{V}(\mathbf{y})$.
(3) $\tilde{V}$ is $\mathcal{R}-$invariant, i.e., $\tilde{V}(R^*\mathbf{y}) = \tilde{V}(\mathbf{y})$.

Remark 2.2. In physics experiments, honeycomb lattices typically are generated by the interference of three laser beams. For a concrete example of such a potential, see, e.g., [1, 3].

Next, we consider the Schrödinger operator

(2.2) $$H = -\Delta + V_{\mathrm{per}}(\mathbf{y}), \quad \mathbf{y} \in \mathbb{R}^2,$$

where V_{per} is assumed to be a smooth honeycomb lattice. Bloch-Floquet theory consequently asserts that the spectrum of H is given by (see [30]):

$$\sigma(H) = \bigcup_{m \in \mathbb{N}} E_m,$$

where $E_m = \{\mu_m(\mathbf{k}) : \mathbf{k} \in Y^*\}$ is called the m-th energy band, or Bloch band. The eigenvalues $\mu_m(\mathbf{k})$ are thereby obtained through the $\mathbf{k}-$pseudo periodic eigenvalue problem (1.2). The associated eigenfunctions $\Phi_m(\cdot; \mathbf{k}) \in H^2_{\mathrm{loc}}(\mathbb{R}^2)$ are $\mathbf{k}-$pseudo periodic, and usually referred to as Bloch waves. They form, for every fixed $\mathbf{k} \in Y^*$ a complete orthonormal basis on $L^2(Y)$ where from now on, we denote

$$\langle f, g \rangle_{L^2(Y)} = \frac{1}{|Y|} \int_Y \overline{f(\mathbf{y})} g(\mathbf{y}) \, d\mathbf{y},$$

the associated L^2-inner product. We also note that for any $m \in \mathbb{N}$ there exists a closed subset $I \subset Y^*$ such that the functions $\mu_m^2(k)$ are real analytic functions for all $k \in Y^*/I$, and we have the following condition

$$\mu_{m-1}(\mathbf{k}) < \mu_m(\mathbf{k}) < \mu_{m+1}(\mathbf{k}), \ \mathbf{k} \in Y^*/I.$$

We call E_m an isolated Bloch band if the condition above holds for all $\mathbf{k} \in Y^*$. Lastly, it is known that

$$|I| = |\{\mathbf{k} \in Y^* : \mu_m(\mathbf{k}) = \mu_{m+1}(\mathbf{k})\}| = 0,$$

and it is in this set of measure zero that we encounter what are called band crossings. At such band crossings one does not have differentiability in $\mathbf{k}$ of the eigenvalues and eigenfunctions.

2.2. **Dirac Points.** An important feature of honeycomb lattice potentials is the presence of Dirac points. The following definition is taken from [16]:

Definition 2.3. Let V be a smooth honeycomb lattice potential. Then a vertex $\mathbf{K} = \mathbf{K}_* \in Y^*$ is called a **Dirac point** if the following holds: There exists $m_1 \in \mathbb{N}$, a real number μ_*, and strictly positive numbers, λ and δ, such that:

(1) μ_* is a degenerate eigenvalue of H with associated $\mathbf{K}_*$-pseudo-periodic eigenfunctions.
(2) dim Nullspace$(H - \mu_*) = 2$.
(3) Nullspace$(H - \mu_*) = \text{span}\{\Phi_1, \Phi_2\}$, where $\Phi_1 \in L^2_{\mathbf{K},\tau}$ and $\Phi_2 \in L^2_{\mathbf{K},\overline{\tau}}$.
(4) There exists Lipschitz functions $\mu_\pm(\mathbf{k})$,

$$\mu_{m_1}(\mathbf{k}) = \mu_-(\mathbf{k}), \quad \mu_{m_1+1}(\mathbf{k}) = \mu_+(\mathbf{k}), \quad \mu_{m_1}(\mathbf{K}_*) = \mu_*,$$

and $E_\pm(\mathbf{k})$, defined for $|\mathbf{k} - \mathbf{K}_*| < \delta$, such that

$$\mu_+(\mathbf{k}) - \mu_* = +\lambda|\mathbf{k} - \mathbf{K}_*|(1 + E_+(\mathbf{k}))$$
$$\mu_-(\mathbf{k}) - \mu_* = -\lambda|\mathbf{k} - \mathbf{K}_*|(1 + E_-(\mathbf{k})),$$

where $|E_\pm(\mathbf{k})| < C|\mathbf{k} - \mathbf{K}_*|$ for some $C > 0$.

For later purposes we also recall the following result from [16] which is computed using the Fourier series expansion $\Phi_{1,2}$, spanning the two dimensional eigenspace associated to μ_*.

Proposition 2.4. *Let $\zeta = (\zeta_1, \zeta_2) \in \mathbb{C}^2$ some vector. Then it holds*

$$\langle \Phi_n, \zeta \cdot \nabla \Phi_n \rangle_{L^2(Y)} = 0 \ , \ n = 1, 2,$$
$$2i\langle \Phi_1, \zeta \cdot \nabla \Phi_2 \rangle_{L^2(Y)} = \overline{2i\langle \Phi_2, \zeta \cdot \nabla \Phi_1 \rangle}_{L^2(Y)} = -\overline{\lambda_\#}(\zeta_1 + i\zeta_2),$$
$$2i\langle \Phi_2, \zeta \cdot \nabla \Phi_1 \rangle_{L^2(Y)} = -\lambda_\#(\zeta_1 - i\zeta_2),$$

where $\lambda_\# \in \mathbb{C}$ is defined by

$$\lambda_\# = 3|Y| \sum_{\mathbf{m} \in S} c(\mathbf{m})^2 \begin{pmatrix} 1 \\ i \end{pmatrix} \cdot \mathbf{K}_\mathbf{m}^*.$$

Here $\{c(\mathbf{m})\}_{\mathbf{m} \in S \subset \mathbb{Z}^2}$ denotes the sequence of $L^2_{\mathbf{K}_*,\tau}$ Fourier coefficients of the normalized eigenstate $\Phi_1(\mathbf{x})$ and $\mathbf{K}_\mathbf{m}^* = \mathbf{K}_* + m_1 \mathbf{k}_1 + m_2 \mathbf{k}_2$.

If $\lambda_\# \neq 0$, then (4) in Definition 2.3 above holds with $\lambda = |\lambda_\#|$. For the present paper, we shall thus make the standing assumption:

Assumption 1. $V_{\text{per}} \in C^\infty(\mathbb{R}^2; \mathbb{R})$ *is a smooth honeycomb lattice potential, which admits Dirac points such that $\lambda_\# \neq 0$.*

It is proved in [16], that this assumption is generically satisfied.

3. Multi-scale asymptotic expansions

3.1. **Formal derivation of the Dirac system.** In this section, we shall follow the ideas in [8, 19], and perform a formal multi-scale expansion of the solution to (1.4) under the Assumption 1. To this end, we seek a solution of the form

$$\Psi^\varepsilon(t,\mathbf{x}) \underset{\varepsilon\to 0}{\sim} \Psi^\varepsilon_N(t,\mathbf{x}) := e^{-i\lambda t/\varepsilon} \sum_{n=0}^{N} \varepsilon^n u_n\Big(t,\mathbf{x},\frac{\mathbf{x}}{\varepsilon}\Big), \quad \lambda \in \mathbb{R},$$

where each $u_n(t,\mathbf{x},\cdot)$ is supposed to be $\mathbf{k}-$pseudo periodic with respect to the fast variable $\mathbf{y} = \frac{\mathbf{x}}{\varepsilon}$. From now on, we denote the linear Hamiltonian by

$$(3.1) \qquad\qquad H^\varepsilon = -\varepsilon^2 \Delta + V_{\mathrm{per}}\Big(\frac{\mathbf{x}}{\varepsilon}\Big)$$

and formally plug the ansatz Ψ^ε_N into (1.4). This yields

$$i\varepsilon\partial_t\Psi^\varepsilon_N - H^\varepsilon\Psi^\varepsilon_N - \varepsilon\kappa|\Psi^\varepsilon_N|^2\Psi^\varepsilon_N = e^{-i\lambda(t/\varepsilon)}\sum_{n=0}^{N}\varepsilon^n X_n + \rho(\Psi^\varepsilon_N),$$

where the remainder is

$$(3.2) \qquad\qquad \rho\left(\Psi^\varepsilon_N\right) = e^{-i\lambda(t/\varepsilon)}\sum_{n=N+1}^{3N+1}\varepsilon^n X_n.$$

Introducing the operators

$$L_0 = \lambda - H, \quad L_1 = i\partial_t + 2\nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{y}}, \quad L_2 = \Delta_{\mathbf{x}},$$

with H given by (2.2), we find (after some lengthy calculations) that

$$X_n = L_0 u_n + L_1 u_{n-1} + L_2 u_{n-2} - \kappa\sum_{\substack{j+k+l+1=n\\0\leqslant j,k,l<n}} u_j u_k \overline{u}_l.$$

We can then proceed by solving $X_n = 0$ for all $n \leqslant N$, to obtain an approximate solution Ψ^ε_N, which formally solves the NLS up to an error of order $\mathcal{O}(\varepsilon^{N+1})$. To this end, the leading order equation is $L_0 u_0 = 0$, which means

$$Hu_0 \equiv (-\Delta_{\mathbf{y}} + V_{\mathrm{per}}(\mathbf{y}))u_0 = \lambda u_0.$$

In view of the assumption that u_0 is $\mathbf{k}-$pseudo periodic, this implies that $\lambda = \mu(\mathbf{k})$ is a Bloch eigenvalue. We shall from now on fix $\mathbf{k} = \mathbf{K}_*$ to be a Dirac point satisfying Assumption 1, and denote the associated eigenvalue by $\lambda = \mu_*$. The leading order amplitude u_0 can thus be written as

$$(3.3) \qquad\qquad u_0(t,\mathbf{x},\mathbf{y}) = \sum_{j=1}^{2}\alpha_j(t,\mathbf{x})\Phi_j(\mathbf{y};\mathbf{K}_*),$$

where $\Phi_{1,2}$ span the two-dimensional eigenspace of μ_*, cf. Definition 2.3.

To determine the leading order amplitudes α_1, α_2 we set $X_1 = 0$ to obtain

$$(3.4) \qquad\qquad L_0 u_1 = \kappa|u_0|^2 u_0 - L_1 u_0.$$

Explicitly, the right hand side reads

$$(3.5) \quad \kappa|u_0|^2 u_0 - L_1 u_0 = -i\sum_{j,k,l=1}^{2}\Big(\Phi_j\partial_t\alpha_j - 2i\nabla_{\mathbf{x}}\alpha_j\cdot\nabla_{\mathbf{y}}\Phi_j + i\kappa\alpha_j\overline{\alpha}_k\alpha_l\Phi_j\overline{\Phi}_k\Phi_l\Big).$$

By Fredholm's alternative, a necessary condition for the solvability of (3.4) is that the right hand side $\notin \ker(L_0)$. Denoting by $\mathbb{P}_* = \mathbb{P}^2_*$ the $L^2(Y)-$projection on the spectral subspace corresponding to μ_*, we consequently require

$$\mathbb{P}_*(\kappa|u_0|^2 u_0 - L_1 u_0) = 0,$$

or, more explicitly:

$$\sum_{j,k,l=1}^{2} \left\langle \Phi_m, \Phi_j \partial_t \alpha_j - 2i\nabla_{\mathbf{x}}\alpha_j \cdot \nabla_{\mathbf{y}}\Phi_j + i\kappa\alpha_j\overline{\alpha}_k\alpha_l\Phi_j\overline{\Phi}_k\Phi_l \right\rangle_{L^2(Y)} = 0, \text{ for } m = 1, 2.$$

Applying Proposition 2.4 with $\zeta = \nabla_{\mathbf{x}}\alpha_j \in \mathbb{C}^2$ for $j = 1, 2$, respectively, we obtain the following system of equations

$$\partial_t \alpha_1 + \overline{\lambda}_{\#}\left(\partial_{x_1} + i\partial_{x_2}\right)\alpha_2 + i\sum_{j,k,l=1}^{2} \kappa_{(j,k,l,1)}\alpha_j\overline{\alpha}_k\alpha_l = 0$$

$$\partial_t \alpha_2 + \lambda_{\#}\left(\partial_{x_1} - i\partial_{x_2}\right)\alpha_1 + i\sum_{j,k,l=1}^{2} \kappa_{(j,k,l,2)}\alpha_j\overline{\alpha}_k\alpha_l = 0,$$

where $\lambda_{\#} \neq 0$ is as above, and

$$\kappa_{(j,k,l,m)} = \kappa\left\langle \Phi_m, \Phi_j\overline{\Phi}_k\Phi_l \right\rangle_{L^2(Y)}.$$

The latter can now be evaluated, using symmetry considerations of the action of the operator $\mathcal{R}$, defined in (2.1), when acting onto Bloch eigenfunctions. We recall that $\Phi_1 \in L^2_{\mathbf{K},\tau}, \Phi_2 \in L^2_{\mathbf{K},\overline{\tau}}$ are eigenfunctions for $\mathcal{R}$ such that

$$\mathcal{R}[\Phi_1(\mathbf{y})] = \Phi_1(R^*\mathbf{y}) = \tau\Phi_1(\mathbf{y}), \quad \mathcal{R}[\Phi_2(\mathbf{y})] = \overline{\Phi}_1(-R^*\mathbf{y}) = \overline{\tau}\Phi_2(\mathbf{y}),$$

where $\tau = e^{2\pi i/3}$. To compute the integrals $\left\langle \Phi_m, \Phi_j\overline{\Phi}_k\Phi_l \right\rangle_{L^2(Y)}$ we use the change of coordinates $\mathbf{y} = R^*\mathbf{w}$ and apply the relations above, to obtain:

$$\kappa_{(j,k,l,m)} = \kappa\int_{R(Y)} \overline{\Phi}_m(R^*\mathbf{w})\Phi_j(R^*\mathbf{w})\overline{\Phi}_k(R^*\mathbf{w})\Phi_l(R^*\mathbf{w}) \, d\mathbf{w}$$

$$= \kappa\int_Y \overline{\tau}_m\overline{\Phi}_m(\mathbf{w})\tau_j\Phi_j(\mathbf{w})\overline{\tau}_k\overline{\Phi}_k(\mathbf{w})\tau_l\Phi_l(\mathbf{w}) \, d\mathbf{w} = \tau_j\overline{\tau}_k\tau_l\overline{\tau}_m\kappa_{(j,k,l,m)},$$

so that

$$\kappa_{(j,k,l,m)}\left(1 - C_{(j,k,l,m)}\right) = 0, \quad C_{(j,k,l,m)} = \tau_j\overline{\tau}_k\tau_l\overline{\tau}_m.$$

We consequently find that $\kappa_{(j,k,l,m)}$ vanishes, whenever $C_{(j,k,l,m)} \neq 1$. A computation shows

$$C_{(j,j,j,m)} = \tau_j\overline{\tau}_j\tau_j\overline{\tau}_m = \tau_j\overline{\tau}_m \neq 1 \text{ for } m \neq j,$$
$$C_{(j,k,j,m)} = C_{(k,j,m,j)} = \tau_j^2\overline{\tau}_k\overline{\tau}_m = \tau_k\overline{\tau}_k\overline{\tau}_m = \overline{\tau}_m \neq 1 \text{ for } m = 1, 2,$$
$$C_{(j,j,k,m)} = \tau_j\overline{\tau}_j\tau_k\overline{\tau}_m = \tau_k\overline{\tau}_m \neq 1 \text{ for } k \neq m = j,$$

and we consequently deduce that the only non-vanishing coefficients are

$$b_1 := \kappa_{(1,1,1,1)} = \kappa_{(2,2,2,2)} = \int_Y |\Phi_1(\mathbf{y})|^4 \, d\mathbf{y} = \int_Y |\Phi_2(\mathbf{y})|^4 \, d\mathbf{y},$$

$$b_2 := \kappa_{(1,1,2,2)} = \kappa_{(1,2,2,1)} = \kappa_{(2,2,1,1)} = \kappa_{(2,1,1,2)} = \int_Y |\Phi_1(\mathbf{y})|^2|\Phi_2(\mathbf{y})|^2 \, d\mathbf{y}.$$

In summary, we find the nonlinear Dirac system as announced in (1.6):

$$\begin{cases} \partial_t \alpha_1 + \overline{\lambda}_{\#}\left(\partial_{x_1} + i\partial_{x_2}\right)\alpha_2 + i\kappa\left(b_1|\alpha_1|^2 + 2b_2|\alpha_2|^2\right)\alpha_1 = 0, \\ \partial_t \alpha_2 + \lambda_{\#}\left(\partial_{x_1} - i\partial_{x_2}\right)\alpha_1 + i\kappa\left(b_1|\alpha_2|^2 + 2b_2|\alpha_1|^2\right)\alpha_2 = 0. \end{cases}$$

Obviously, this system needs to be supplemented with initial data $\alpha_{1,0}$, $\alpha_{2,0}$, which we shall, for simplicity, assume to be in the Schwartz space $\mathcal{S}(\mathbb{R}^2)$.

3.2. **Higher order corrections.** Assuming that the leading order amplitudes α_1, α_2 satisfy the nonlinear Dirac system allows us to proceed with our expansion and solve (3.4) for u_1. We obtain a unique solution in the form

$$(3.6) \qquad u_1(t, \mathbf{x}, \mathbf{y}) = \tilde{u}_1(t, \mathbf{x}, \mathbf{y}) + u_1^\perp(t, \mathbf{x}, \mathbf{y}),$$

where $\tilde{u}_1 \in (\ker L_0)$ i.e.

$$(3.7) \qquad \tilde{u}_1(t, \mathbf{x}, \mathbf{y}) = \sum_{j=1}^{2} \beta_j(t, \mathbf{x}) \Phi_j(\mathbf{y}, \mathbf{K}_*)$$

for some yet to be determined amplitudes $\beta_{1,2}$, and

$$(3.8) \qquad u_1^\perp(t, \mathbf{x}, \mathbf{y}) = -L_0^{-1}\big(L_1 u_0 - \kappa|u_0|^2 u_0\big) \in (\ker L_0)^\perp.$$

Here we denote by L_0^{-1} the partial inverse (or partial resolvent) of L_0, i.e.

$$L_0^{-1} = (1 - \mathbb{P}_*)(\mu_* - H)^{-1}(1 - \mathbb{P}_*).$$

Note that at $t = 0$, the function $u_1^\perp(0, \mathbf{x}, \mathbf{y})$ cannot be chosen, but rather has to be determined from the initial data $\alpha_{0,1}, \alpha_{0,2}$ according to the formula above.

Proceeding further, we need to determine the amplitudes β_1, β_2 by setting $X_2 = 0$, i.e.

$$L_0 u_2 = -L_1 u_1 - L_2 u_0 + \kappa\big(u_0^2 \overline{u}_1 + 2|u_0|^2 u_1\big).$$

By the same arguments as before, we obtain the following system of linear, inhomogeneous Dirac equations for $\beta_{1,2}$ as the corresponding solvability condition:

$$(3.9) \quad \begin{cases} \partial_t \beta_1 + \overline{\lambda}_\# \big(\partial_{x_1} + i\partial_{x_2}\big)\beta_2 + i\displaystyle\sum_{j,k,l=1}^{2} \kappa_{(j,k,l,1)}\Big(\alpha_j \overline{\beta}_k \alpha_l + 2\beta_j \overline{\alpha}_k \alpha_l\Big) = i\Theta_1 \\[2mm] \partial_t \beta_2 + \lambda_\# \big(\partial_{x_1} - i\partial_{x_2}\big)\beta_1 + i\displaystyle\sum_{j,k,l=1}^{2} \kappa_{(j,k,l,2)}\Big(\alpha_j \overline{\beta}_k \alpha_l + 2\beta_j \overline{\alpha}_k \alpha_l\Big) = i\Theta_2, \end{cases}$$

where the right hand side source terms can be written as

$$(3.10) \qquad \Theta_n = \Delta\alpha_n + \langle \Phi_n, L_1 u_1^\perp \rangle_{L^2(Y)} - \kappa\langle \Phi_n, (u_0 \overline{u}_1^\perp + 2\overline{u}_0 u_1^\perp)u_0 \rangle_{L^2(Y)}.$$

We have the freedom to choose vanishing initial data $\beta_{1,2}(0, \mathbf{x}) = 0$ for the system (3.9), which nevertheless will have a non-vanishing solution due to the source terms. In summary, this allows us to write

$$u_2(t, \mathbf{x}, \mathbf{y}) = \tilde{u}_2(t, \mathbf{x}, \mathbf{y}) + u_2^\perp(t, \mathbf{x}, \mathbf{y}),$$

where as before $\tilde{u}_2 \in (\ker L_0)$ and $u_2^\perp \in (\ker L_0)^\perp$. The latter is obtained by elliptic inversion on $(\ker L_0)^\perp$, i.e.

$$(3.11) \qquad u_2(t, \mathbf{x}, \mathbf{y}) = -L_0^{-1}\Big(L_1 u_1 + L_2 u_0 - \kappa\big(u_0^2 \overline{u}_1 + 2|u_0|^2 u_1\big)\Big).$$

All higher order terms u_n can then be determined analogously. However, since we are mainly interested in deriving the nonlinear Dirac system for the leading order amplitudes $\alpha_{1,2}$, we shall see that it is sufficient to stop our expansion at $N = 2$. Note that in order to satisfy $X_2 = 0$, one does not need to determine the amplitudes within $\tilde{u}_2 \in (\ker L_0)$, which will simplify our treatment below.

4. Mathematical framework for the approximate solution

4.1. Local well-posedness of the Dirac equations.

We aim to make the formal multi-scale expansion of the foregoing section mathematically rigorous. To do so, we shall in a first step construct a unique local in-time solution with sufficient smoothness for the nonlinear Dirac model (1.6). To this end, we will work in the Banach space $X = C([0,T]; H^s(\mathbb{R}^2))^2$ for $s > 1$, endowed with the norm

$$\|\mathbf{u}\|_X = \sup_{0 \leqslant t \leqslant T} \|\mathbf{u}(t)\|_{H^s} \equiv \sup_{0 \leqslant t \leqslant T} \left(\|u_1(t)\|_{H^s}^2 + \|u_2(t)\|_{H^s}^2 \right)^{1/2},$$

where $\mathbf{u} = (u_1, u_2)$. For the sake of notation, let us rewrite (1.6) in a more compact form. Namely, let $\boldsymbol{\alpha} = (\alpha_1, \alpha_2)$ and define $\sigma_1^\# := P_\# \sigma_1$, $\sigma_2^\# := P_\# \overline{\sigma_2}$ where $\sigma_{1,2}$ are the Pauli spin matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

and

$$P_\# = \begin{pmatrix} \overline{\lambda_\#} & 0 \\ 0 & \lambda_\# \end{pmatrix}.$$

Then (1.6) can be written as

$$(4.1) \qquad i\partial_t \boldsymbol{\alpha} = -i(\boldsymbol{\sigma} \cdot \nabla)\boldsymbol{\alpha} + \kappa \mathbf{F}(\boldsymbol{\alpha}), \quad \boldsymbol{\alpha}_{|t=0} = \boldsymbol{\alpha}_0(\mathbf{x}),$$

where we denote

$$(\boldsymbol{\sigma} \cdot \nabla) := \sigma_1^\# \partial_{x_1} + \sigma_2^\# \partial_{x_2}$$

and $\mathbf{F}(\boldsymbol{\alpha})$ is the nonlinearity discussed in the following lemma.

Lemma 4.1. *Consider the function*

$$G(\alpha_1, \overline{\alpha}_1, \alpha_2, \overline{\alpha}_2) = \frac{b_1}{2} \left(|\alpha_1|^4 + |\alpha_2|^4 \right) + 2b_2 |\alpha_1|^2 |\alpha_2|^2,$$

with $\boldsymbol{\alpha} = (\alpha_1, \alpha_2) \in H^s(\mathbb{R}^2)^2$. *Then, the nonlinear vector field* $\mathbf{F}(\boldsymbol{\alpha}) = \begin{pmatrix} \partial_{\overline{\alpha}_1} G \\ \partial_{\overline{\alpha}_2} G \end{pmatrix}$ *is a map from* $H^s(\mathbb{R}^2)^2 \to H^s(\mathbb{R}^2)^2$ *for any* $s > 1$.

Proof. We note that for $s > 1$, $H^s(\mathbb{R}^2) \hookrightarrow L^\infty(\mathbb{R}^2)$ is a commutative algebra such that

$$\forall f, g \in H^s(\mathbb{R}^2), \ \|fg\|_{H^s} \leqslant C_s \|f\|_{H^s} \|g\|_{H^s}.$$

This directly yields

$$\|\mathbf{F}(\boldsymbol{\alpha})\|_{H^s} \leqslant \left(b_1 + 2b_2 \right) C_s^2 \|\boldsymbol{\alpha}\|_{H^s}^3 < \infty.$$

$\square$

Using the Fourier transform, we also have that the linear time-evolution governed by the (strongly continuous) Dirac group

$$(U(t)f)(\mathbf{x}) = e^{t\sigma \cdot \nabla} f(\mathbf{x}) \equiv \mathcal{F}^{-1}\left(e^{-it\boldsymbol{\sigma} \cdot \boldsymbol{\xi}} \widehat{f}(\boldsymbol{\xi}) \right)(\mathbf{x}),$$

satisfies $\|U(t)\mathbf{u}\|_{H^s} = \|\mathbf{u}\|_{H^s}$ for all $s \in \mathbb{R}$ and all $t \in \mathbb{R}$. Together with the foregoing lemma, this can be used to prove the following local well-posedness result.

Proposition 4.2. *For any* $\boldsymbol{\alpha}_0 \in \mathcal{S}(\mathbb{R}^2)^2$ *there exists a time* $T > 0$ *and a unique maximal solution* $\boldsymbol{\alpha} \in C\left([0,T]; H^s(\mathbb{R}^2)\right) \cap C^1\left((0,T); H^{s-1}(\mathbb{R}^2)\right)^2$ *for all* $s > 1$ *to (4.1). Moreover, it holds*

$$\|\alpha_1(t, \cdot)\|_{L^2} + \|\alpha_2(t, \cdot)\|_{L^2} = \text{ const. } \forall t \in [0, T).$$

Proof. This follows by a fixed point argument applied to Duhamel's formulation of (4.1), i.e.

$$(4.2) \qquad \boldsymbol{\alpha}(t) = U(t)\boldsymbol{\alpha}_0 - i\kappa \int_0^t U(t - \tau)\mathbf{F}(\mathbf{u}(\tau))d\tau =: (\Phi\boldsymbol{\alpha})(t).$$

Indeed, using Lemma 4.1, one easily sees that for any $\boldsymbol{\alpha}_0 \in \mathcal{S}(\mathbb{R}^2)^2$ such that $\|\boldsymbol{\alpha}_0\|_{H^s} \leqslant R$, the functional $\Phi : X \to X$ is a contraction mapping on $K = \{\boldsymbol{\alpha} \in X : \|\boldsymbol{\alpha}\|_X \leqslant 2R\}$, provided $T = \dfrac{1}{8(b_1 + 2b_2)R^2 C_s^2} > 0$. The asserted regularity in time then follows by differentiating the equation. Finally, the identity for mass conservation is obtained by multiplying the equations by $\overline{\alpha}_j$, integrating and taking the imaginary part. $\qquad\square$

With this result in hand, we can also get local well-posedness for the inhomogeneous linear Dirac equation (3.9) on the same time-interval, i.e., we have

$$(4.3) \qquad \boldsymbol{\beta} \in C\big([0, T); H^{s-2}(\mathbb{R}^2)\big)^2,$$

in view of the fact that the coefficients $\boldsymbol{\alpha} \in C([0, T); L^\infty(\mathbb{R}^2))^2$ and the source terms satisfy $\boldsymbol{\theta} \in C\big([0, T); H^{s-2}(\mathbb{R}^2)\big)^2$. The latter can be seen from (3.10) which involves the Laplacian of u_0 and thus we lose two derivatives.

Remark 4.3. The main obstacle to obtain global well-posedness of the nonlinear Dirac equation (4.1), is the fact that the corresponding energy does not have a definite sign, i.e.,

$$E(t) = \mathrm{Im} \left(\overline{\lambda_\#} \int_{\mathbb{R}^2} \alpha_2(\partial_{x_1} + i\partial_{x_2})\overline{\alpha}_1 \, d\mathbf{x} \right) - \frac{\kappa}{4} \int_{\mathbb{R}^2} b_1|\boldsymbol{\alpha}|^2 + 4b_2|\alpha_1|^2|\alpha_2|^2 \, d\mathbf{x}.$$

So far, the existence of global in time solutions is thus restricted to small initial data cases, see, e.g., [4, 13, 14, 24] and the references therein. The fact that (4.1) is also massless, is an additional complication, as the spectral subspaces for the corresponding free Dirac operator are no longer separated (a fact that requires considerable more care than the case with nonzero mass).

4.2. **Estimates on the approximate solution and the remainder.** Formally, the approximate solution Ψ_N^ε derived in Section 3 solves the NLS up to errors of order $\mathcal{O}(\varepsilon^{N+1})$. To make this error estimate rigorous on time-scales of order $\mathcal{O}(1)$, we shall prove a nonlinear stability result in Section 5 below. The latter will require us to work with an approximate solution of order $N > 1$. We consequently need to work (at least) with Ψ_2^ε. As was already remarked above, though, in order to solve the NLS up to reminders of $\mathcal{O}(\varepsilon^2)$, one does not need to determine the highest order amplitudes within $\tilde{u}_2 \in (\ker L_0)$. We shall thus set them identically equal to zero and work with an approximate solution of the following form

$$\begin{aligned} \Psi_{\mathrm{app}}^\varepsilon(t, \mathbf{x}) &= e^{-i\mu_* t/\varepsilon}\Big(u_0 + \varepsilon u_1 + \varepsilon^2 u_2\Big)\Big(t, \mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\Big) \\ (4.4) \qquad\qquad &= e^{-i\mu_* t/\varepsilon} \sum_{j=1}^2 \big(\alpha_j + \varepsilon\beta_j\big)(t, \mathbf{x})\Phi_j\Big(\frac{\mathbf{x}}{\varepsilon}; \mathbf{K}_*\Big) + \varepsilon^j u_j^\perp\Big(t, \mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\Big), \end{aligned}$$

where $\alpha_{1,2} \in C\big([0, T); H^s(\mathbb{R}^2)\big)$ and $\beta_{1,2} \in C\big([0, T); H^{s-2}(\mathbb{R}^2)\big)$ for $s > 1$, are the leading and first order amplitudes guaranteed to exist by the results of the previous subsection. The term of order $\mathcal{O}(\varepsilon^2)$ within this approximation is solely determined by elliptic inversion and thereby depends on the two lower order terms.

Since $\Psi_{\mathrm{app}}^\varepsilon$ involves the highly oscillatory Bloch eigenfuntions, we cannot expect to obtain uniform (in ε) estimates in the usual Sobolev spaces $H^s(\mathbb{R}^2)$. We shall therefore work in the following ε-scaled spaces, as used in [8, 19].

Definition 4.4. Let $s \in \mathbb{Z}$, $0 < \varepsilon \leqslant 1$, and $f \in H_\varepsilon^s(\mathbb{R}^2)$ and define the $H_\varepsilon^s(\mathbb{R}^2)-$norm by

$$\|f\|_{H_\varepsilon^s}^2 := \sum_{|\gamma| \leqslant s} \|(\varepsilon \partial_x)^\gamma f\|_{L^2}^2.$$

A family f^ε is bounded in $H_\varepsilon^s(\mathbb{R}^2)$ whenever

$$\sup_{0 < \varepsilon \leqslant 1} \|f^\varepsilon\|_{H_\varepsilon^s} < \infty.$$

We note that in $H_\varepsilon^s(\mathbb{R}^2)$ the following Gagliardo-Nirenberg inequality holds

(4.5) $$\forall s > 1 \; \exists C_\infty > 0 : \; \|f\|_{L^\infty} \leqslant C_\infty \varepsilon^{-1} \|f\|_{H_\varepsilon^s},$$

where the "bad" factor ε^{-1} is obtained by scaling.

The following proposition then collects the necessary regularity estimates for our approximate solution and its corresponding remainder.

Proposition 4.5. *Let V_{per} satisfy Assumption 1 and choose $S \in (4, \infty)$ such that $S > s + 3$ for any $s > 1$. Let*

$$\boldsymbol{\alpha} \in C\Big([0,T), H^S(\mathbb{R}^2)\Big)^2, \quad \boldsymbol{\beta} \in C\Big([0,T), H^{S-2}(\mathbb{R}^2)\Big)^2$$

be the solutions to (non-)linear Dirac systems (4.1) and (3.9), respectively. Then, the approximate solution $\Psi_{\mathrm{app}}^\varepsilon(t, \cdot)$, given in (4.4), satisfies the following estimates for all $t \in [0, T)$ and for any $|\gamma| < s - 1$:

$$\|(\varepsilon \partial)^\gamma \Psi_{\mathrm{app}}^\varepsilon(t, \cdot)\|_{L^\infty} \leqslant C_a, \quad \|\Psi_{\mathrm{app}}^\varepsilon(t, \cdot)\|_{H_\varepsilon^s} \leqslant C_b, \quad \|\rho(\Psi_{\mathrm{app}}^\varepsilon)(t, \cdot)\|_{H_\varepsilon^s} \leqslant C_r \varepsilon^3.$$

with $C_a, C_b, C_r > 0$ independent of ε.

Proof. To prove the estimates of the lemma, we need to first establish the regularity of $u_n(t) = u_n\big(t, \mathbf{x}, \mathbf{y}\big)$ for $n = 0, 1, 2$. We note first that Assumption 1 implies that the eigenfunctions $\Phi_j(\cdot; \mathbf{K}^*) \in C^\infty(\overline{Y})$, $j = 1, 2$, cf. [30]. We shall then prove the following, preliminary estimate for $t \in [0, T)$

(4.6) $$u_n(t) \in H^{S-3}(\mathbb{R}^2) \times C_{\mathbf{K}_*}^\infty(\overline{Y}), \quad n = 0, 1, 2,$$

where $C_{\mathbf{K}_*}^\infty(\overline{Y})$ is the space of smooth $\mathbf{K}_*-$pseudo-periodic functions on $\overline{Y}$. To this end, we have for $t \in [0, T)$ that

$$u_0(t) \in H^S(\mathbb{R}^2) \times C_{\mathbf{K}_*}^\infty(\overline{Y}),$$

due to (3.3) and Proposition 4.2. Next, recall that u_1 is of the form (3.6) with $\tilde{u}_1$ and $u_1^\perp$ given by (3.7) and (3.8), respectively. In view of (3.7) and (4.3), we directly infer

$$\tilde{u}_1(t) \in H^{S-2}(\mathbb{R}^2) \times C_{\mathbf{K}_*}^\infty(\overline{Y}).$$

Moreover, since $L_0^{-1} : L^2(Y) \to H_{\mathrm{per}}^2(Y)$ and $L_1 = i\partial_t + 2\nabla x \cdot \nabla_y$ it follows from (3.4) that

$$u_1^\perp(t) \in H^{S-1}(\mathbb{R}^2) \times C_{\mathbf{K}_*}^\infty(\overline{Y}),$$

and thus

$$u_1(t) \in H^{S-2}(\mathbb{R}^2) \times C_{\mathbf{K}_*}^\infty(\overline{Y}),$$

since $H^s(\mathbb{R}^2) \subset H^{s-1}(\mathbb{R}^2)$ for all $s > 0$. Lastly, we recall that u_2 has the same type of structure with $u_2^\perp$ given by (3.11). Similarly, as before it then follows that

$$u_2(t) \in H^{S-3}(\mathbb{R}^2) \times C_{\mathbf{K}_*}^\infty(\overline{Y}).$$

In summary, this yields (4.6) which implies $u_n\Big(t, \cdot, \frac{\cdot}{\varepsilon}\Big) \in H_\varepsilon^{S-3}\big(\mathbb{R}^2\big)$ for $n = 0, 1, 2$. Hence it follows that for any $s > 1$

$$u_n\Big(t, \cdot, \frac{\cdot}{\varepsilon}\Big) \in H_\varepsilon^s\big(\mathbb{R}^2\big), \quad n = 0, 1, 2,$$

whenever $S - 3 > s$ which gives the condition stated above. Moreover it follows that

$$\|\Psi_{\mathrm{app}}(t, \cdot)\|_{H_\varepsilon^s} \leqslant \sum_{n=0}^{2} \varepsilon^n \|u_n\|_{H_\varepsilon^s} \leqslant \sum_{n=0}^{2} \|u_n\|_{H_\varepsilon^{S-3}} = C_b.$$

Having established this, our next step is to prove the first inequality of the lemma. It suffices to show that there exists a constant $C_0 > 0$ such that

$$(4.7) \qquad \left\| (\varepsilon\partial)^\gamma u_0 \left(t, \cdot, \frac{\cdot}{\varepsilon}\right) \right\|_{L^\infty} \leqslant C_0$$

holds for all $\varepsilon \in (0, 1), |\gamma| < s - 1$, and $t \in [0, T)$. Since u_0 is of the form (3.3), we need only to show that

$$\left\| (\varepsilon\partial)^\gamma \left(\alpha_{1,2}(t, \cdot) \Phi_{1,2} \left(\frac{\cdot}{\varepsilon}; \mathbf{K}_* \right) \right) \right\|_{L^\infty} \leqslant C,$$

where C is a constant independent of epsilon. By the Leibniz rule one has

$$(\varepsilon\partial)^\gamma \left(\alpha_{1,2}(t, \mathbf{x}) \Phi_{1,2} \left(\frac{\mathbf{x}}{\varepsilon}; \mathbf{K}_* \right) \right) = \sum_{|\sigma| \leqslant |\gamma|} \binom{|\gamma|}{\sigma} (\varepsilon\partial)^\sigma \alpha_{1,2}(t, \mathbf{x}) \cdot (\varepsilon\partial)^{\sigma-\gamma} \Phi_{1,2} \left(\frac{\mathbf{x}}{\varepsilon}; \mathbf{K}_* \right),$$

and we can thus estimate

$$\left\| (\varepsilon\partial)^\gamma \left(\alpha_{1,2}(t, \cdot) \Phi_{1,2} \left(\frac{\cdot}{\varepsilon}; \mathbf{K}_* \right) \right) \right\|_{L^\infty}$$

$$\leqslant C_1 \sum_{|\sigma| \leqslant |\gamma|} \left\| (\varepsilon\partial)^\sigma \alpha_{1,2}(t, \cdot) \right\|_{L^\infty} \left\| (\varepsilon\partial)^{\sigma-\gamma} \Phi_{1,2} \left(\frac{\cdot}{\varepsilon}; \mathbf{K}_* \right) \right\|_{L^\infty}$$

$$\leqslant C_2 \left\| \Phi_{1,2} \left(\cdot; \mathbf{K}_* \right) \right\|_{C_{\mathbf{K}_*}^{|\gamma|}} \sum_{|\sigma| \leqslant |\gamma|} \left\| \partial^\sigma \alpha_{1,2}(t, \cdot) \right\|_{L^\infty}$$

$$\leqslant C_3 \left\| \alpha_{1,2}(t, \cdot) \right\|_{H^{2+|\gamma|}} \leqslant C,$$

where the second to last inequality follows by Sobolev embedding. Hence (4.7) follows by the triangle inequality. For $n = 1, 2$, one invokes (4.5) directly to obtain

$$\| (\varepsilon\partial)^\gamma u_n \left(t, \cdot, \frac{\cdot}{\varepsilon} \right) \|_{L^\infty} \leqslant C_\infty \varepsilon^{-1} \|u_n\|_{H_\varepsilon^{m+|\gamma|}} \leqslant \varepsilon^{-1} \|u_n\|_{H^s} \leqslant \varepsilon^{-1} C_n,$$

provided that $m > 1$ and $m + |\gamma| \leqslant s$, which implies $|\gamma| < s - 1$. The desired inequality then follows, since

$$\| (\varepsilon\partial)^\gamma \Psi_{\mathrm{app}}^\varepsilon(t, \cdot) \|_{L^\infty} \leqslant C_0 + \sum_{n=1}^{2} \varepsilon^{n-1} \left\| (\varepsilon\partial)^\gamma u_n \left(t, \cdot, \frac{\cdot}{\varepsilon} \right) \right\|_{L^\infty} \leqslant C_a,$$

where C_a is a constant independent of epsilon. One notices that the last inequality follows from the fact that for $n = 3, \ldots, 7$: $X_n \in H_\varepsilon^s(\mathbb{R}^2)$ and so

$$\|\rho(\Psi_{\mathrm{app}})(t, \cdot)\|_{H_\varepsilon^s} \leqslant \sum_{n=3}^{7} \varepsilon^n \|X_n\|_{H_\varepsilon^s} \leqslant C_r \varepsilon^3.$$

$\square$

With these estimates at hand, we can now prove the stability of our approximation.

5. Nonlinear stability of the approximation

Before we prove the nonlinear stability of our approximation, we recall that it was proved in [19], that the linear Schrödinger group

$$(5.1) \qquad\qquad S^\varepsilon(t) := e^{-iH^\varepsilon t/\varepsilon}$$

generated by the periodic Hamiltonian H^ε defined in (3.1) satisfies

$$(5.2) \qquad \|S^\varepsilon(t)f\|_{H^s_\varepsilon} \leqslant C_s\|f\|_{H^s_\varepsilon} \text{ for all } t \in \mathbb{R} \text{ and all } \varepsilon \in (0,1),$$

where $C_s > 0$ is independent of ε. To this end, one uses the fact that V_{per} is assumed to be smooth and periodic (as guaranteed by Assumption 1). Using this, it is straightforward to obtain the following basic well-posedness result for nonlinear Schrödinger equations.

Lemma 5.1. *Let V_{per} satisfy Assumption 1 and $\Psi^\varepsilon_0 \in H^s_\varepsilon(\mathbb{R}^2)$, for $s > 1$. Then there exists a $T^\varepsilon > 0$ and a unique solution $\Psi^\varepsilon \in C([0,T^\varepsilon); H^s_\varepsilon(\mathbb{R}^2))$ to the initial value problem* (1.4).

Proof. In view of (5.2), the proof is a straightforward extension of the one given in, e.g., [29, Proposition 3.8] for the case without periodic potential. $\square$

Remark 5.2. Note that this result does not preclude the possibility that $T^\varepsilon \to 0_+$, as $\varepsilon \to 0_+$. However, it will be a by-product of our main theorem below that this is not the case (at least not for the class of initial data considered in this work).

As a final preparatory step, we recall the following Moser-type lemma proved in [28, Lemma 8.1.1].

Lemma 5.3. *Let $R > 0$, $s \in [0, \infty)$, and $\mathcal{N}(z) = \kappa|z|^2 z$ with $\kappa \in \mathbb{R}$. Then there exists a $C_s = C_s(R, s, d, \kappa)$ such that if f satisfies*

$$\|(\varepsilon\partial)^\gamma f\|_{L^\infty} \leqslant R \quad \forall |\gamma| \leqslant s,$$

and g satisfies

$$\|g\|_{L^\infty} \leqslant R,$$

then

$$\|\mathcal{N}(f+g) - \mathcal{N}(f)\|_{H^s_\varepsilon} \leqslant C_s\|g\|_{H^s_\varepsilon}$$

In contrast to other estimates (e.g., Schauder etc.), the above result has the advantage to result in a linear bound on the nonlinearity, a fact we shall use in the proof below. Indeed, we are now in the position to prove our main result.

Theorem 5.4. *Let V_{per} satisfy Assumption 1, let $\boldsymbol{\alpha} \in C([0,T], H^S(\mathbb{R}^2))^2$ be a solution to* (1.4) *and $\boldsymbol{\beta} \in C([0,T], H^{S-2}(\mathbb{R}^2))^2$ be a solution to* (3.9) *for some $S > s + 3$ with $s > 1$. Finally, assume that there is a $c > 0$ such that the initial data Ψ^ε_0 of* (1.4) *satisfies*

$$\left\| \Psi^\varepsilon_0 - \left(u_0 + \varepsilon u_1\right)\left(0, \cdot, \frac{\cdot}{\varepsilon}\right) \right\|_{H^s_\varepsilon} \leqslant c\varepsilon^2.$$

Then, for any $T_* \in [0,T)$ there exists an $\varepsilon_0 = \varepsilon_0(T_*) \in (0,1)$ and a constant $C > 0$, such that for all $\varepsilon \in (0, \varepsilon_0)$, the solution $\Psi^\varepsilon \in C([0, T_*); H^s_\varepsilon(\mathbb{R}^2))$ of (1.4) *exists and moreover*

$$\sup_{0 \leqslant t \leqslant T_*} \left\| \Psi^\varepsilon(t, \cdot) - e^{-i\mu_* t/\varepsilon}\left(u_0 + \varepsilon u_1\right)\left(t, \cdot, \frac{\cdot}{\varepsilon}\right) \right\|_{H^s_\varepsilon} \leqslant C\varepsilon^2.$$

Proof. Consider the difference in the exact and approximate solution

$$\varphi^\varepsilon = \Psi^\varepsilon - \Psi^\varepsilon_{\mathrm{app}},$$

then $\varphi^\varepsilon(t, \mathbf{x})$ satisfies

$$i\partial_t \varphi^\varepsilon = \frac{1}{\varepsilon} H^\varepsilon \varphi^\varepsilon + \left(\mathcal{N}(\Psi^\varepsilon_{\mathrm{app}} + \varphi^\varepsilon) - \mathcal{N}(\Psi^\varepsilon_{\mathrm{app}})\right) - \frac{1}{\varepsilon}\rho(\Psi^\varepsilon_{\mathrm{app}}), \quad \varphi^\varepsilon_{|t=0} = \varphi^\varepsilon_0,$$

where H^ε is defined in (3.1), the nonlinearity is $\mathcal{N}(z) = \kappa |z|^2 z$, and $\rho(\Psi^\varepsilon_{\mathrm{app}})$ is the remainder obtained in (3.2) for $N = 2$. We denote $w^\varepsilon(t) := \|\varphi^\varepsilon(t)\|_{H^s_\varepsilon}$ and first note by assumption that

$$w^\varepsilon(0) \equiv \|\varphi^\varepsilon_0\|_{H^s_\varepsilon} \leqslant \left\|\Psi^\varepsilon(0, \cdot) - (u_0 + \varepsilon u_1)\left(0, \cdot, \frac{\cdot}{\varepsilon}\right)\right\|_{H^s_\varepsilon} + \varepsilon^2 \|u_2^\perp(0, \cdot)\|_{H^s_\varepsilon} \leqslant \tilde{c}\varepsilon^2,$$

for some constant $\tilde{c} \in \mathbb{R}$. We shall prove that there exists $\tilde{C} > 0$, $\varepsilon_0 \in (0, 1)$, such that for all $\varepsilon \in (0, \varepsilon_0]$ that $w^\varepsilon(t) \leqslant \tilde{C}\varepsilon^2$ for $t \in [0, T_*]$.

To this end, we rewrite the equation above using Duhamel's principle, i.e.

$$\varphi^\varepsilon(t) = S^\varepsilon(t)\varphi^\varepsilon_0 - i \int_0^t S^\varepsilon(t - \tau)\left(\mathcal{N}(\Psi^\varepsilon_{\mathrm{app}}(\tau) + \varphi^\varepsilon(\tau)) - \mathcal{N}(\Psi^\varepsilon_{\mathrm{app}}(\tau))\right) d\tau$$

$$+ \frac{i}{\varepsilon} \int_0^t S^\varepsilon(t - \tau)\rho(\Psi^\varepsilon_{\mathrm{app}}(\tau)) \, d\tau,$$

where $S^\varepsilon(t)$ is the Schrödinger group (5.1). Now, using the propagation estimate (5.2), together with the estimate on the remainder stated in Proposition 4.5, we obtain

$$w^\varepsilon(t) \leqslant C_l(\tilde{c} + C_r T_*)\varepsilon^2 + C_l \int_0^t \left\|\mathcal{N}(\Psi^\varepsilon_{\mathrm{app}}(\tau) + \varphi^\varepsilon(\tau)) - \mathcal{N}(\Psi^\varepsilon_{\mathrm{app}}(\tau))\right\|_{H^s_\varepsilon} d\tau.$$

for all $t \leqslant T_*$.

Set $\tilde{C} := C_l(\tilde{c} + C_r T_*)e^{C_l C_s T_*}$ and choose $M > \max\{\tilde{c}, \tilde{C}\}$ such that $M\varepsilon^2 > \tilde{c}\varepsilon^2 \geqslant w^\varepsilon(0)$. Since $w^\varepsilon(t)$ is continuous in time, there exists, for every $\varepsilon \in (0, 1)$, a positive time $t^\varepsilon_M > 0$, such that $w^\varepsilon(t) \leqslant \varepsilon^2 M$ for $t \leqslant t^\varepsilon_M$. The Gagliardo-Nirenberg inequality (4.5) then yields for $s > 1$

$$\|\varphi^\varepsilon(t)\|_{L^\infty} \leqslant \varepsilon^{-1} C_\infty \|\varphi^\varepsilon(t)\|_{H^s_\varepsilon} = \varepsilon^{-1} C_\infty w^\varepsilon(t) \leqslant \varepsilon C_\infty M$$

for $t \leqslant t^\varepsilon_M$. Hence there exists an $\varepsilon_0 \in (0, 1)$, such that

$$\|\varphi^\varepsilon(t)\|_{L^\infty} \leqslant C_a,$$

for $\varepsilon \in (0, \varepsilon_0]$ and $t \leqslant t^\varepsilon_M$. By Proposition 4.5 we also have

$$\|(\varepsilon\partial)^\gamma \Psi_{\mathrm{app}}(t, \cdot)\|_{L^\infty} \leqslant C_a$$

for $|\gamma| \leqslant s - 1, \varepsilon \in (0, 1)$, and $t < T$. Thus we are in a position to apply the Moser-type Lemma 5.3 with $R = C_a$ to obtain

$$w^\varepsilon(t) \leqslant C_l(c + C_r T_*)\varepsilon^2 + C_l C_s \int_0^t w^\varepsilon(\tau) \, d\tau, \text{ for } \varepsilon \in (0, \varepsilon_0] \text{ and } t \leqslant t^\varepsilon_M.$$

Gronwall's lemma then yields

$$w^\varepsilon(t) \leqslant C_l(\tilde{c} + C_r T_*)\varepsilon^2 e^{C_l C_s t} \leqslant \tilde{C}\varepsilon^2 < M \text{ for all } \varepsilon \in (0, \varepsilon_0] \text{ and } t \leqslant T_*.$$

Hence for any choice of T_*, by continuity, we may extend further in time in that $t^\varepsilon_M \geq T_*$, and so we have proved that for any $T_* < T$:

$$\sup_{0 \leqslant t \leqslant T_*} w^\varepsilon(t) \equiv \sup_{0 \leqslant t \leqslant T_*} \|\Psi^\varepsilon(t, \cdot) - \Psi^\varepsilon_{\mathrm{app}}(t, \cdot)\|_{H^s_\varepsilon} \leqslant \tilde{C}\varepsilon^2.$$

Another triangle inequality, then yields the desired result. $\qquad\square$

This theorem implies the approximation result announced in (1.5), uniformly on finite time-intervals bounded by the local existence time of (4.1), provided the initial data is sufficiently well prepared, i.e. up to errors of order $\mathcal{O}(\varepsilon^2)$.

Remark 5.5. Unfortunately, our proof requires us to work with an approximate solution of order $\mathcal{O}(\varepsilon^2)$, in which we need to control also the first order corrector $\propto u_1$. In turn, this requires the initial data to be somewhat better than one would like it to be. The reason for this is the scaling factor ε^{-1} appearing in the Gagliardo-Nirenberg inequality (4.5). It is conceivable that this is merely a technical issue which can be overcome by the use of a different functional framework. For example, the authors in [11, 12] work in a Wiener-type space for the Bloch-transformed solution and its approximation.

6. The case of Hartree nonlinearities

In this section, we shall briefly discuss the case of NLS with Hartree nonlinearity, i.e., instead of (1.4), we consider

$$(6.1) \quad i\varepsilon\partial_t\Psi^\varepsilon = -\varepsilon^2\Delta\Psi^\varepsilon + V_{\mathrm{per}}\left(\frac{\mathbf{x}}{\varepsilon}\right)\Psi^\varepsilon + \varepsilon\kappa\left(\frac{1}{|\cdot|}*|\Psi^\varepsilon|^2\right)\Psi^\varepsilon, \quad \Psi^\varepsilon_{|t=0} = \Psi^\varepsilon_0(\mathbf{x}).$$

This model describes the (semi-classical) dynamics of electrons inside a graphene layer, under the influence of a self-consistent electric field.

We again seek an asymptotic expansion of the form

$$\Psi^\varepsilon(t,\mathbf{x}) \underset{\varepsilon\to 0}{\sim} e^{-it\mu_*/\varepsilon} \sum_{n=0}^{2} \varepsilon^n u_n\left(t,\mathbf{x},\frac{\mathbf{x}}{\varepsilon}\right),$$

where as before the u_n are assumed to be $\mathbf{k}-$pseudo periodic with respect to the fast variable. By the same procedure as in Section 3, we obtain that

$$u_0(t,\mathbf{x},\mathbf{y}) = \sum_{j=1}^{2} \alpha_j(t,\mathbf{x})\Phi_j(\mathbf{y};\mathbf{K}_*).$$

Plugging this into the Hartree nonlinearity, yields the following nonlinear potential

$$V^\varepsilon(t,\mathbf{x}) = \frac{1}{|\cdot|} * \sum_{j,k=1}^{2} \left(\alpha_j\overline{\alpha}_k\Phi_j\overline{\Phi}_k\right)\left(t,\cdot,\frac{\cdot}{\varepsilon}\right),$$

which unfortunately does not directly exhibit the required two-scale structure. However, we shall prove the following averaging result.

Lemma 6.1. Let $\alpha_j(t,\mathbf{x}) \in H^s(\mathbb{R}^2)$, for $s > 1$, then

$$\lim_{\varepsilon\to 0} V^\varepsilon(t,\mathbf{x}) = \left(\frac{1}{|\cdot|} * \left(|\alpha_1|^2 + |\alpha_2|^2\right)\right)(t,\mathbf{x}).$$

Proof. We recall that Bloch eigenfunctions concentrated at a Dirac point have a Fourier series expansion of the following form, cf. [16]:

$$\Phi_1(\mathbf{y},\mathbf{K}^*) = \sum_{\mathbf{m}\in\mathbb{Z}^2} c(\mathbf{m})e^{i\mathbf{K}^*_{\mathbf{m}}\cdot\mathbf{x}},$$

$$\Phi_2(\mathbf{x},\mathbf{K}^*) = \overline{\Phi}_1(-\mathbf{x},\mathbf{K}^*) = \sum_{\mathbf{m}\in\mathbb{Z}^2} \overline{c}(\mathbf{m})e^{i\mathbf{K}^*_{\mathbf{m}}\cdot\mathbf{x}},$$

where

$$\mathbf{K}^*_{\mathbf{m}} = \mathbf{K}_* + m_1\mathbf{k}_1 + m_2\mathbf{k}_2 = \mathbf{K}_* + \mathbf{k}_{\mathbf{m}}.$$

By orthogonality and Parseval's identity one finds the following relations to be used below

$$\sum_{\mathbf{m}\in\mathbb{Z}^2} |c(\mathbf{m})|^2 = \int_Y |\Phi_1(\mathbf{x})|^2 \, d\mathbf{x} = 1,$$

$$\sum_{\mathbf{m}\in\mathbb{Z}^2} c(\mathbf{m})^2 = \langle c(\mathbf{m}), \overline{c}(\mathbf{m})\rangle_{\ell_2(\mathbb{Z}^2)} = \int_Y \Phi_1(\mathbf{x})\overline{\Phi}_2(\mathbf{x}) \, d\mathbf{x} = 0,$$

$$\sum_{\mathbf{m}\in\mathbb{Z}^2} \overline{c}(\mathbf{m})^2 = \langle \overline{c}(\mathbf{m}), c(\mathbf{m})\rangle_{\ell_2(\mathbb{Z}^2)} = \int_Y \Phi_2(\mathbf{x})\overline{\Phi}_1(\mathbf{x}) \, d\mathbf{x} = 0.$$

Next, we decompose

$$V^\varepsilon = V_1^\varepsilon + V_2^\varepsilon \equiv \frac{1}{|\cdot|} * \sum_{j=1}^2 |\alpha_j|^2 |\Phi_j|^2 + \frac{1}{|\cdot|} * \sum_{j\neq k} \alpha_j \overline{\alpha}_k \Phi_j \overline{\Phi}_k.$$

Explicitly, we find

$$V_1^\varepsilon(t,\mathbf{x}) = \int_{\mathbb{R}^2} \left(\left|\alpha_1(t,\boldsymbol{\eta})\right|^2 \left|\Phi_1\left(\frac{\boldsymbol{\eta}}{\varepsilon}\right)\right|^2 + \left|\alpha_2(t,\boldsymbol{\eta})\right|^2 \left|\Phi_2\left(\frac{\boldsymbol{\eta}}{\varepsilon}\right)\right|^2 \right) \frac{d\boldsymbol{\eta}}{|\mathbf{x}-\boldsymbol{\eta}|}$$

$$= \sum_{\mathbf{m},\mathbf{m}'\in\mathbb{Z}^2} c(\mathbf{m})\overline{c}(\mathbf{m}') \int_{\mathbb{R}^2} \left(\left|\alpha_1(t,\boldsymbol{\eta})\right|^2 + \left|\alpha_2(t,\boldsymbol{\eta})\right|^2 \right) e^{i(\mathbf{k}_{\mathbf{m}-\mathbf{m}'}\cdot\boldsymbol{\eta})/\varepsilon} \frac{d\boldsymbol{\eta}}{|\mathbf{x}-\boldsymbol{\eta}|},$$

and similarly,

$$V_2^\varepsilon(t,\mathbf{x}) =$$

$$= \int_{\mathbb{R}^2} \left(\alpha_1(t,\boldsymbol{\eta})\overline{\alpha}_2(t,\boldsymbol{\eta})\Phi_1\left(\frac{\boldsymbol{\eta}}{\varepsilon}\right)\overline{\Phi}_2\left(\frac{\boldsymbol{\eta}}{\varepsilon}\right) + \overline{\alpha}_1(t,\boldsymbol{\eta})\alpha_2(t,\boldsymbol{\eta})\overline{\Phi}_1\left(\frac{\boldsymbol{\eta}}{\varepsilon}\right)\Phi_2\left(\frac{\boldsymbol{\eta}}{\varepsilon}\right) \right) \frac{d\boldsymbol{\eta}}{|\mathbf{x}-\boldsymbol{\eta}|}$$

$$= \sum_{\mathbf{m},\mathbf{m}'\in\mathbb{Z}^2} c(\mathbf{m})c(\mathbf{m}') \int_{\mathbb{R}^2} \alpha_1(t,\boldsymbol{\eta})\overline{\alpha}_2(t,\boldsymbol{\eta}) e^{i(\mathbf{k}_{\mathbf{m}-\mathbf{m}'}\cdot\boldsymbol{\eta})/\varepsilon} \frac{d\boldsymbol{\eta}}{|\mathbf{x}-\boldsymbol{\eta}|}$$

$$+ \sum_{\mathbf{m},\mathbf{m}'\in\mathbb{Z}^2} \overline{c}(\mathbf{m})\overline{c}(\mathbf{m}') \int_{\mathbb{R}^2} \overline{\alpha}_1(t,\boldsymbol{\eta})\alpha_2(t,\boldsymbol{\eta}) e^{-i(\mathbf{k}_{\mathbf{m}-\mathbf{m}'}\cdot\boldsymbol{\eta})/\varepsilon} \frac{d\boldsymbol{\eta}}{|\mathbf{x}-\boldsymbol{\eta}|}.$$

Now, since the kernel $\frac{1}{|\cdot|}$ in two spatial dimensions is integrable at the origin and since $\alpha_{1,2}\in L^2(\mathbb{R}^2)\cap L^\infty(\mathbb{R}^2)$, the Riemann-Lebesgue lemma implies that, as $\varepsilon\to 0$, all ε−oscillatory terms vanish, i.e. all terms for which $\mathbf{m}\neq\mathbf{m}'$. In view of the above identities for the Fourier coefficients we thus find

$$\lim_{\varepsilon\to 0} V_1^\varepsilon(t,\mathbf{x}) = \sum_{\mathbf{m}\in\mathbb{Z}^2} |c(\mathbf{m})|^2 \int_{\mathbb{R}^2} \left(\left|\alpha_1(t,\boldsymbol{\eta})\right|^2 + \left|\alpha_2(t,\boldsymbol{\eta})\right|^2 \right) \frac{d\boldsymbol{\eta}}{|\mathbf{x}-\boldsymbol{\eta}|}$$

$$= \left(\frac{1}{|\cdot|} * \left(\left|\alpha_1\right|^2 + \left|\alpha_2\right|^2 \right) \right)(t,\mathbf{x}),$$

whereas

$$\lim_{\varepsilon\to 0} V_2^\varepsilon(t,\mathbf{x}) = \sum_{\mathbf{m}\in\mathbb{Z}^2} c(\mathbf{m})^2 \int_{\mathbb{R}^2} \alpha_1(t,\boldsymbol{\eta})\overline{\alpha}_2(t,\boldsymbol{\eta}) \frac{d\boldsymbol{\eta}}{|\mathbf{x}-\boldsymbol{\eta}|}$$

$$+ \sum_{\mathbf{m}\in\mathbb{Z}^2} \overline{c}(\mathbf{m})^2 \int_{\mathbb{R}^2} \overline{\alpha}_1(t,\boldsymbol{\eta})\alpha_2(t,\boldsymbol{\eta}) \frac{d\boldsymbol{\eta}}{|\mathbf{x}-\boldsymbol{\eta}|} = 0,$$

since both sums vanish individually. $\qquad\square$

We therefore expect that as $\varepsilon \to 0$, the dynamics of WKB waves spectrally localized around $\mathbf{K}_*$ are governed by the following Dirac-Hartree system:

$$\begin{cases} \partial_t \alpha_1 + \overline{\lambda}_\# \big(\partial_{x_1} + i\partial_{x_2}\big)\alpha_2 = -i\kappa\bigg(\frac{1}{|\cdot|} * \Big(\big|\alpha_1\big|^2 + \big|\alpha_2\big|^2\Big)\bigg)\alpha_1, \\[2ex] \partial_t \alpha_2 + \lambda_\# \big(\partial_{x_1} - i\partial_{x_2}\big)\alpha_1 = -i\kappa\bigg(\frac{1}{|\cdot|} * \Big(\big|\alpha_1\big|^2 + \big|\alpha_2\big|^2\Big)\bigg)\alpha_2, \end{cases}$$

The Cauchy problem for this system has been rigorously studied in [21] as an ad-hoc model for electrons in graphene (see also [22, 25] for related results). Our analysis above indicates, that this is indeed the correct model and we believe that a fully rigorous proof can be achieved along the same lines as in the case of a cubic nonlinearity. However, a rigorous averaging argument for the required second order approximate solution would require considerably more work, a direction we do not want to pursue here.

Remark 6.2. Let us finally note that while the Hartree nonlinearity is equivalent to a coupling with a Poisson equation $-\Delta V = |\Psi^\varepsilon|^2$ in three spatial dimensions, this is no longer the case in 2D. If one were to pursue the coupled system instead of (6.1), the effective model obtained would be a Dirac-Poisson system as studied in [10].

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