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Waves in Honeycomb Structures

Charles L. Fefferman Michael I. Weinstein

Abstract

We review recent work of the authors on the non-relativistic Schrödinger equation with a honeycomb lattice potential, V . In particular, we summarize results on (i) the existence of Dirac points, conical singularities in dispersion surfaces of $H_V = -\Delta + V$ and (ii) the two-dimensional Dirac equations, as the large (but finite) time effective system of equations governing the evolution $e^{-iH_V t}\psi_0$, for data ψ_0 , which is spectrally localized near a Dirac point. We conclude with a formal derivation and discussion of the effective large time evolution for the nonlinear Schrödinger - Gross Pitaevskii equation for small amplitude initial conditions, ψ_0 . The effective dynamics are governed by a nonlinear Dirac system.

1. Introduction

There has been intense interest within the fundamental and applied physics communities in the propagation of waves in honeycomb structures. Two areas where such structures have been explored extensively are (i) condensed matter physics and (ii) photonics:

1. Graphene, a single atomic layer of carbon atoms, is a two-dimensional structure with carbon atoms located at the sites of a honeycomb structure with remarkable electronic properties; see, for example, the survey articles [13, 14].
2. Photonic / electro-magnetic propagation (linear and nonlinear) has been studied in dielectric honeycomb structures [9, 15, 3, 17].

The basic mathematical model is a wave equation, defined on the 2-dimensional plane with a medium whose material properties vary periodically according to a honeycomb pattern: Schrödinger's equation with honeycomb lattice potential, in

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the quantum setting, and Maxwell's equations, with honeycomb structured dielectric parameters, in the electromagnetic setting.

We focus on the time-evolution of the Schrödinger equation

$$i\partial_t\psi = (-\Delta + V(\mathbf{x}))\psi = H_V\psi, \quad (1.1)$$

where $V(\mathbf{x})$ is a smooth, real-valued and periodic potential, defined on \mathbb{R}^2 , with period lattice Λ . Denote by Ω , a choice of elementary period cell of $V(\mathbf{x})$. We are interested in properties of the time-evolution, which relate directly to the special symmetry of the honeycomb lattice. To represent the time evolution operator, $e^{-iH_V t}$, we quickly review the basic Floquet-Bloch spectral theory of periodic potentials.

Consider the family of \mathbf{k} - pseudo-periodic eigenvalue problems:

$$H_V \Phi(\mathbf{x}; \mathbf{k}) = \mu \Phi(\mathbf{x}; \mathbf{k}), \quad \mathbf{x} \in \mathbb{R}^2, \quad (1.2)$$

$$\Phi(\mathbf{x} + \mathbf{v}; \mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{v}} \Phi(\mathbf{x}; \mathbf{k}), \quad \mathbf{v} \in \Lambda. \quad (1.3)$$

We introduce the family of \mathbf{k} - pseudo-periodic L^2 functions, $L_{\mathbf{k}}^2$:

$$L_{\mathbf{k}}^2 = \left\{ f \in L^2(\Omega) : f(\mathbf{x} + \mathbf{v}) = e^{i\mathbf{k}\cdot\mathbf{v}} f(\mathbf{x}), \quad \mathbf{v} \in \Lambda \right\}.$$

Denote by

$$\Lambda_h = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2, \quad \text{where } \mathbf{v}_1 = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, \quad \mathbf{v}_2 = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{1}{2} \end{pmatrix}$$

the period lattice of the regular honeycomb structure; see Figure 1.1.

In (1.2)-(1.3), \mathbf{k} - varies in the Brillouin zone, \mathcal{B} , a choice of fundamental cell in the dual period lattice, Λ^* . For honeycomb lattice potentials,

$$\Lambda_h^* = \mathbb{Z}\mathbf{k}_1 \oplus \mathbb{Z}\mathbf{k}_2, \quad \text{where } \mathbf{k}_1 = \frac{4\pi}{\sqrt{3}} \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}, \quad \mathbf{k}_2 = \frac{4\pi}{\sqrt{3}} \begin{pmatrix} \frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix},$$

and \mathcal{B} can be chosen to be a regular hexagon, centered at the origin. The vertices of \mathcal{B} fall into two equivalence class: points of \mathbf{K} type and points of \mathbf{K}' type, which alternate around the perimeter of \mathcal{B} ; see Figure 1.2.

An equivalent spectral problem with periodic boundary conditions may be obtained by setting $\Phi(\mathbf{x}; \mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} p(\mathbf{x}; \mathbf{k})$. Then, $p(\mathbf{x}; \mathbf{k})$, $\mathbf{k} \in \mathcal{B}$, is Λ - periodic in \mathbf{x} and satisfies boundary value problem:

$$H_V(\mathbf{k})p(\mathbf{x}; \mathbf{k}) = \mu p(\mathbf{x}; \mathbf{k}), \quad \mathbf{x} \in \mathbb{R}^2, \quad (1.4)$$

$$p(\mathbf{x} + \mathbf{v}; \mathbf{k}) = p(\mathbf{x}; \mathbf{k}), \quad \mathbf{v} \in \Lambda, \quad (1.5)$$

where

$$H_V(\mathbf{k}) \equiv -(\nabla + i\mathbf{k})^2 + V(\mathbf{x}). \quad (1.6)$$

For each $\mathbf{k} \in \mathcal{B}$, the spectrum of $H_V(\mathbf{k})$ is discrete, consisting of real eigenvalues:

$$\mu_1(\mathbf{k}) \leq \mu_2(\mathbf{k}) \leq \cdots \leq \mu_b(\mathbf{k}) \leq \cdots$$

(listed with multiplicities), with corresponding eigenfunctions $p_b(\mathbf{x}; \mathbf{k})$, $b \geq 1$. As \mathbf{k} varies over \mathcal{B} , $\mu_b(\mathbf{k})$ sweeps out a closed real interval, $\mu_b(\mathcal{B})$. The spectrum of H_V is the union of these intervals:

$$\text{spectrum}(H_V) = \bigcup_{b \geq 1} \mu_b(\mathcal{B}) \quad (1.7)$$

The Floquet-Bloch modes $\Phi_b(\mathbf{x}; \mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} p_b(\mathbf{x}; \mathbf{k})$, $b \geq 1$ are complete in the sense that for any $f \in L^2(\mathbb{R}^2)$

$$f(\mathbf{x}) - \sum_{1 \leq b \leq N} \int_{\mathcal{B}} \langle \Phi_b(\cdot; \mathbf{k}), f(\cdot) \rangle_{L^2(\mathbb{R}^2)} \Phi_b(\mathbf{x}; \mathbf{k}) d\mathbf{k} \rightarrow 0 \quad (1.8)$$

in $L^2(\mathbb{R}^2)$ as $N \uparrow \infty$. The solution of the initial value problem for time-dependent Schrödinger equation, (1.1), with initial data $\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x})$, has the representation:

$$e^{-iHt} \psi_0 = \sum_{b \geq 1} \int_{\mathcal{B}} e^{-i\mu_b(\mathbf{k})t} \langle \Phi_b(\cdot; \mathbf{k}), \psi_0(\cdot) \rangle_{L^2(\mathbb{R}^2)} \Phi_b(\mathbf{x}; \mathbf{k}) d\mathbf{k}. \quad (1.9)$$

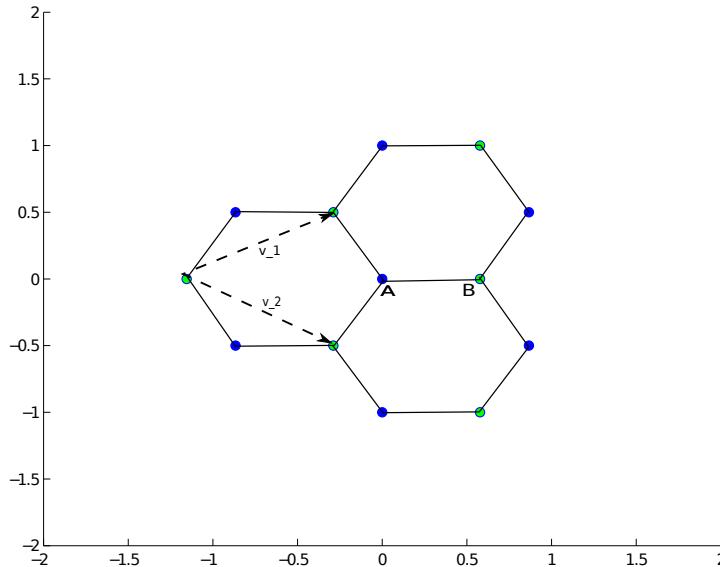


Figure 1.1: Part of the honeycomb structure, \mathbf{H} . \mathbf{H} is the union of two sub-lattices $\Lambda_{\mathbf{A}} = \mathbf{A} + \Lambda_h$ (blue) and $\Lambda_{\mathbf{B}} = \mathbf{B} + \Lambda_h$ (green). The lattice vectors $\{\mathbf{v}_1, \mathbf{v}_2\}$ generate Λ_h .

An understanding of the time-dynamics (1.9) requires, in particular, a detailed understanding of the functions $\mu_b(\mathbf{k})$, $b \geq 1$. These are called *band dispersion functions* of H_V . The graphs $\mathbf{k} \mapsto \mu_b(\mathbf{k})$ are called the *dispersion surfaces* of H_V .

Let's now introduce the class of potentials that interests us. For f defined on \mathbb{R}^2 let

$$\mathcal{R}[f](\mathbf{x}) \equiv f(R^* \mathbf{x}), \quad (1.10)$$

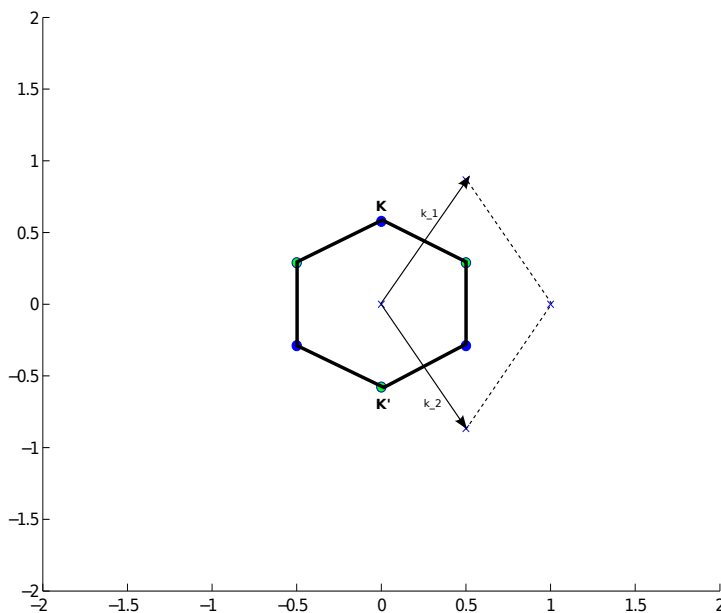


Figure 1.2: Brillouin zone, \mathcal{B} , and dual basis $\{\mathbf{k}_1, \mathbf{k}_2\}$. \mathbf{K} and \mathbf{K}' are labeled. Other vertices of \mathcal{B}_h obtained via application of R , rotation by $2\pi/3$.

where R is the 2×2 rotation matrix, which clockwise-rotates a vector by an angle of $2\pi/3$.

Definition 1.1 (Honeycomb lattice potentials). Let V be real-valued and $V \in C^\infty(\mathbb{R}^2)$. V is a *honeycomb lattice potential* if there exists $\mathbf{x}_0 \in \mathbb{R}^2$ such that $\tilde{V}(\mathbf{x}) = V(\mathbf{x} - \mathbf{x}_0)$ has the following properties:

1. \tilde{V} is Λ_h -periodic, *i.e.* $\tilde{V}(\mathbf{x} + \mathbf{v}) = \tilde{V}(\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^2$ and $\mathbf{v} \in \Lambda_h$.
2. \tilde{V} is even or inversion-symmetric, *i.e.* $\tilde{V}(-\mathbf{x}) = \tilde{V}(\mathbf{x})$.
3. \tilde{V} is \mathcal{R} -invariant, *i.e.*

$$\mathcal{R}[\tilde{V}](\mathbf{x}) \equiv \tilde{V}(R^*\mathbf{x}) = \tilde{V}(\mathbf{x}),$$

where, R^* is the counter-clockwise rotation matrix by $2\pi/3$, *i.e.* $R^* = R^{-1}$.

Thus, a honeycomb lattice potential is smooth, Λ_h -periodic and, with respect to some origin of coordinates, both inversion symmetric and \mathcal{R} -invariant.

In this article we summarize recent results of the authors on the spectral properties of H_V and properties of the evolution operator, $e^{-iH_V t}$, where V denotes a honeycomb lattice potential. In section 2 we describe results on the existence of conical singularities in the dispersion surfaces of honeycomb lattice potentials for quasi-momenta located at the vertices of \mathcal{B} . In section 3 we consider the initial value problem for the non-relativistic Schrödinger equation, (1.1), with a honeycomb lattice potential. We study the evolution for initial conditions which are spectrally

localized about a vertex (\mathbf{K} - type or \mathbf{K}' - type point) of \mathcal{B} and show that the large, but finite, time-evolution is effectively governed by the constant coefficient two-dimensional Dirac equation. Finally in section 4 we remark on some open problems concerning the relation of the nonlinear Schrödinger / Gross-Pitaevskii equation and the two-dimensional nonlinear Dirac equation.

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2. Dirac points

In this section we discuss results of the authors in [7] on the conical singularities, so-called *Dirac points*, in the dispersion surfaces of H_V , where V is a honeycomb lattice potential.

A key property of honeycomb lattice potentials, V is that if \mathbf{K}_* denotes any vertex of \mathcal{B} , then we have the commutation relation:

$$[\mathcal{R}, H_V(\mathbf{K}_*)] = 0. \quad (2.1)$$

Since \mathcal{R} has eigenvalues $1, \tau$ and $\bar{\tau}$, it is natural to the split $L_{\mathbf{K}_*}^2$, the space of \mathbf{K}_* -pseudo-periodic functions, into the direct sum:

$$L_{\mathbf{K}_*}^2 = L_{\mathbf{K}_*,1}^2 \oplus L_{\mathbf{K}_*,\tau}^2 \oplus L_{\mathbf{K}_*,\bar{\tau}}^2, \quad (2.2)$$

where $L_{\mathbf{K}_*,\sigma}^2$ are invariant eigen-subspaces of \mathcal{R} , *i.e.* for $\sigma = 1, \tau, \bar{\tau}$, where $\tau = \exp(2\pi i/3)$, and

$$L_{\mathbf{K}_*,\sigma}^2 = \left\{ g \in L_{\mathbf{K}_*}^2 : \mathcal{R}g = \sigma g \right\}. \quad (2.3)$$

We next give a precise definition of a Dirac point.

Definition 2.1. Let $V(\mathbf{x})$ be a smooth, real-valued, even (inversion symmetric) and periodic potential on \mathbb{R}^2 . Denote by \mathcal{B} , the Brillouin zone. We call $\mathbf{K} \in \mathcal{B}$ a *Dirac point* if the following holds: There exist an integer $b_1 \geq 1$, a real number μ_* , and strictly positive numbers, λ and δ , such that:

1. μ_* is a degenerate eigenvalue of H with \mathbf{K} - pseudo-periodic boundary conditions.
2. $\dim \text{Nullspace}(H - \mu_* I) = 2$
3. $\text{Nullspace}(H - \mu_* I) = \text{span}\left\{ \Phi_1(\mathbf{x}), \Phi_2(\mathbf{x}) \right\}$, where $\Phi_1 \in L_{\mathbf{K},\tau}^2$ ($\mathcal{R}\Phi_1 = \tau\Phi_1$) and $\Phi_2(\mathbf{x}) = \overline{\Phi_1(-\mathbf{x})} \in L_{\mathbf{K},\bar{\tau}}^2$ ($\mathcal{R}\Phi_2 = \bar{\tau}\Phi_2$).
4. There exist Lipschitz functions $\mu_{\pm}(\mathbf{k})$,

$$\mu_{b_1}(\mathbf{k}) = \mu_-(\mathbf{k}) \quad \mu_{b_1+1}(\mathbf{k}) = \mu_+(\mathbf{k}), \quad \mu_{\pm}(\mathbf{K}) = \mu_*$$

and $E_{\pm}(\mathbf{k})$, defined for $|\mathbf{k} - \mathbf{K}| < \delta$, and \mathbf{k} - pseudo-periodic eigenfunctions of H : $\Phi_{\pm}(\mathbf{x}; \mathbf{k})$, with corresponding eigenvalues $\mu_{\pm}(\mathbf{k})$ such that

$$\begin{aligned} \mu_+(\mathbf{k}) - \mu(\mathbf{K}) &= +\lambda |\mathbf{k} - \mathbf{K}| (1 + E_+(\mathbf{k})) \quad \text{and} \\ \mu_-(\mathbf{k}) - \mu(\mathbf{K}) &= -\lambda |\mathbf{k} - \mathbf{K}| (1 + E_-(\mathbf{k})), \end{aligned} \quad (2.4)$$

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

Remark 2.1. In [7] we prove the following

Proposition 2.2. Suppose conditions 1., 2. and 3. of Definition 2.1 hold and denote by $\{c(\mathbf{m})\}_{\mathbf{m} \in \mathcal{S}}$ the sequence of $L^2_{\mathbf{K},\tau}$ Fourier-coefficients of $\Phi_1(\mathbf{x})$. Define the sum

$$\lambda_{\sharp} \equiv \sum_{\mathbf{m} \in \mathcal{S}} c(\mathbf{m})^2 \begin{pmatrix} 1 \\ i \end{pmatrix} \cdot \mathbf{K}_*^{\mathbf{m}} . \quad (2.5)$$

Here, the index set $\mathcal{S} \subset \mathbb{Z}^2$ is defined in [7]. If $\lambda_{\sharp} \neq 0$, then 4. of Definition 2.1 holds (see (2.4)) with $\lambda = |\lambda_{\sharp}|$.

Therefore Dirac points are found by verifying conditions 1., 2. and 3. of Definition 2.1 and the additional (non-degeneracy) condition: $\lambda_{\sharp} \neq 0$. We use this characterization to prove the following result, Theorem 5.1 of [7], concerning the existence of Dirac points for Schrödinger operators with a generic honeycomb lattice potentials:

Theorem 2.1. Let $V(\mathbf{x})$ honeycomb lattice potential. Assume further that the Fourier coefficient of V , $V_{1,1}$, is non-vanishing, *i.e.*

$$V_{1,1} \equiv \int_{\Omega} e^{-i(k_1+k_2)\cdot\mathbf{y}} V(\mathbf{y}) d\mathbf{y} \neq 0 . \quad (2.6)$$

Consider the one-parameter family of honeycomb Schrödinger operators defined by:

$$H^{(\epsilon)} \equiv -\Delta + \epsilon V(\mathbf{x}) . \quad (2.7)$$

There exists a countable and closed set $\tilde{\mathcal{C}} \subset \mathbb{R}$ such that for all $\epsilon \notin \tilde{\mathcal{C}}$, the vertices, \mathbf{K}_* , of \mathcal{B}_h are Dirac points in the sense of Definition 2.1.

More specifically, the following holds for $\epsilon \notin \tilde{\mathcal{C}}$: There exists $b_1 \geq 1$ such that $\mu_* \equiv \mu_{b_1}^{\epsilon}(\mathbf{K}_*) = \mu_{b_1+1}^{\epsilon}(\mathbf{K}_*)$ is a \mathbf{K}_* - pseudo-periodic eigenvalue of multiplicity two where

1. μ_*^{ϵ} is an $L^2_{\mathbf{K},\tau}$ - eigenvalue of $H^{(\epsilon)}$ of multiplicity one, and corresponding eigenfunction, $\Phi_1^{\epsilon}(\mathbf{x})$.

μ_*^{ϵ} is an $L^2_{\mathbf{K},\bar{\tau}}$ - eigenvalue of $H^{(\epsilon)}$ of multiplicity one, with corresponding eigenfunction, $\Phi_2^{\epsilon}(\mathbf{x}) = \overline{\Phi_1^{\epsilon}(-\mathbf{x})}$.

μ_*^{ϵ} is not an $L^2_{\mathbf{K},1}$ - eigenvalue of $H^{(\epsilon)}$.

2. There exist $\delta_{\epsilon} > 0$, $C_{\epsilon} > 0$ and Floquet-Bloch eigenpairs: $(\Phi_+^{\epsilon}(\mathbf{x}; \mathbf{k}), \mu_+^{\epsilon}(\mathbf{k}))$ and $(\Phi_-^{\epsilon}(\mathbf{x}; \mathbf{k}), \mu_-^{\epsilon}(\mathbf{k}))$, and Lipschitz continuous functions, $E_{\pm}^{\epsilon}(\mathbf{k})$, defined for $|\mathbf{k} - \mathbf{K}_*| < \delta_{\epsilon}$, such that

$$\begin{aligned} \mu_+^{\epsilon}(\mathbf{k}) - \mu^{\epsilon}(\mathbf{K}_*) &= + |\lambda_{\sharp}^{\epsilon}| |\mathbf{k} - \mathbf{K}_*| \left(1 + E_+^{\epsilon}(\mathbf{k}) \right) \quad \text{and} \\ \mu_-^{\epsilon}(\mathbf{k}) - \mu^{\epsilon}(\mathbf{K}_*) &= - |\lambda_{\sharp}^{\epsilon}| |\mathbf{k} - \mathbf{K}_*| \left(1 + E_-^{\epsilon}(\mathbf{k}) \right) , \end{aligned}$$

where

$$\lambda_{\sharp}^{\epsilon} \equiv \sum_{\mathbf{m} \in \mathcal{S}} c(\mathbf{m}, \mu_*^{\epsilon}, \epsilon)^2 \begin{pmatrix} 1 \\ i \end{pmatrix} \cdot \mathbf{K}_*^{\mathbf{m}} \neq 0 \quad (2.8)$$

is given in terms of $\{c(\mathbf{m}, \mu_*^{\epsilon}, \epsilon)\}_{\mathbf{m} \in \mathcal{S}}$, the $L^2_{\mathbf{K},\tau}$ - Fourier coefficients of $\Phi^{\epsilon}(\mathbf{x}; \mathbf{K}_*)$.

Furthermore, $|E_{\pm}^{\epsilon}(\mathbf{k})| \leq C_{\epsilon} |\mathbf{k} - \mathbf{K}_*|$. Thus, in a neighborhood of the point $(\mathbf{k}, \mu) = (\mathbf{K}_*, \mu_*^{\epsilon}) \in \mathbb{R}^3$, the dispersion surface is closely approximated by a circular *cone*.

3. There exists $\epsilon^0 > 0$, such that for all $\epsilon \in (-\epsilon^0, \epsilon^0) \setminus \{0\}$
 - (i) $\epsilon V_{1,1} > 0 \implies$ conical intersection of 1st and 2nd dispersion surfaces
 - (ii) $\epsilon V_{1,1} < 0 \implies$ conical intersection of 2nd and 3rd dispersion surfaces .

Remark 2.2. In a forthcoming article, we present a general analytic perturbation theory of deformed honeycomb lattice Hamiltonians, for perturbations which commute with inversion composed with complex conjugation. Conical (Dirac) points persist for small perturbations of this type, although the conical singularities typically perturb away from the vertices of \mathcal{B} . These results extend those of [7] and, in particular, include the case of a linearly strained honeycomb structure.

Remarks on the proof of Theorem 2.1 [7]: Following the strategy outlined in Remark 2.1, we first show, for all ϵ sufficiently small and non-zero, by a Lyapunov-Schmidt reduction, that the degenerate, multiplicity three eigenvalue of the Laplacian with \mathbf{K}_* - pseudo-periodic boundary condition, splits into a multiplicity two eigenvalue and a multiplicity one eigenvalue, with associated \mathcal{R} - invariant eigenspaces. Next, we must show the persistence of this degenerate multiplicity two subspace as ϵ is increased without bound. To continue to ϵ large we introduce a globally-defined analytic function, $\mathcal{E}(\mu, \epsilon)$, whose zeros, counting multiplicity, are the eigenvalues of $H^{(\epsilon)}$. Eigenvalues occur where an operator $I + \mathcal{C}(\mu, \epsilon)$, $\mathcal{C}(\mu, \epsilon)$ compact, is singular. Since $\mathcal{C}(\mu, \epsilon)$ is not trace-class but is Hilbert-Schmidt, we work with $\mathcal{E}(\mu, \epsilon) = \det_2(I + \mathcal{C}(\mu, \epsilon))$, a renormalized determinant. Next $\mathcal{E}(\mu, \epsilon)$ and $\lambda_{\sharp}^{\epsilon}$ are studied using techniques of complex function theory to establish the existence of Dirac points for arbitrary real values of ϵ , except possibly for a countable closed subset, $\tilde{\mathcal{C}} \subset \mathbb{R}$. The origin of this exceptional set is a topological obstruction to the existence of continuous choice of eigenvector as parameters are varied.

Previous analyses of honeycomb lattice structures are based upon extreme limit models: the tight-binding / infinite contrast limit (see, for example, [18, 13, 11]) in which the potential is taken to be concentrated at lattice points or edges of a graph; in this limit, the dispersion relation has an explicit analytical expression, or the weak-potential limit, treated by formal perturbation theory in [9, 2] and rigorously in [8].

3. Evolution of wave packets and the two-dimensional Dirac equation

From the previous section, we see that generic honeycomb Hamiltonians, H_V , have Dirac points, about which some band dispersion surface is *approximately* that of a two-dimensional wave equation with wave speeds $\pm|\lambda_{\sharp}|$. Thus, initial conditions which are spectrally localized about a Dirac point, should evolve *approximately* according to a constant coefficient hyperbolic PDE with wave speeds $\pm|\lambda_{\sharp}|$. In this section we summarize results deriving the appropriate wave equation and its time-scale of validity in terms of the degree of spectral localization, δ , about a Dirac point, \mathbf{K}_* .

A general solution of the time-dependent Schrödinger equation, constrained to the degenerate 2-dimensional eigenspace associated with eigenvalue, $\mu_* = \mu(\mathbf{K}_*)$, associated with the Dirac point, \mathbf{K}_* , is of the form

$$\psi(\mathbf{x}, t) = e^{-i\mu_* t} (\alpha_1 \Phi_1(\mathbf{x}) + \alpha_2 \Phi_2(\mathbf{x})), \quad (3.1)$$

where α_1 and α_2 are arbitrary constants.

Consider now a *wave packet* initial condition, which is spectrally concentrated near \mathbf{K}_* :

$$\begin{aligned}\psi^\delta(\mathbf{x}, 0) &= \psi_0^\delta(\mathbf{x}) = \delta \left(\alpha_{10}(\delta\mathbf{x}) \Phi_1(\mathbf{x}) + \alpha_{20}(\delta\mathbf{x}) \Phi_2(\mathbf{x}) \right) \\ &= \delta \left(\alpha_{10}(\delta\mathbf{x}) p_1(\mathbf{x}) + \alpha_{20}(\delta\mathbf{x}) p_2(\mathbf{x}) \right) e^{i\mathbf{K}_* \cdot \mathbf{x}}\end{aligned}\quad (3.2)$$

Here, $\delta > 0$ is a small parameter. We assume $\alpha_{10}(\mathbf{X})$ and $\alpha_{20}(\mathbf{X})$ are Schwartz functions of \mathbf{X} . This assumption can be weakened considerably without difficulty. The overall factor of δ in (3.2) is not essential (the problem is linear), but is inserted so that ψ_0^δ has $L^2(\mathbb{R}^2)$ -norm (and $H^2(\mathbb{R}^2)$ -norms) of order of magnitude one.

We seek solutions of (1.1), (3.2) in the form:

$$\psi^\delta(\mathbf{x}, t) = e^{-i\mu_* t} \left(\sum_{j=1}^2 \delta \alpha_j(\delta\mathbf{x}, \delta t) \Phi_j(\mathbf{x}) + \eta^\delta(\mathbf{x}, t) \right). \quad (3.3)$$

$$\text{where } \eta^\delta(\mathbf{x}, 0) = 0, \quad \alpha_j(\mathbf{X}, 0) = \alpha_{j0}(\mathbf{X}), \quad j = 1, 2 \quad (3.4)$$

to ensure the initial condition (3.2).

The goal is to show that the Schrödinger equation (1.1) has a solution of the form (3.3) with an error term, $\eta^\delta(\mathbf{x}, t)$, which satisfies

$$\sup_{0 \leq t \leq \rho \delta^{-2+\varepsilon_1}} \|\eta^\delta(\cdot, t)\|_{H^s(\mathbb{R}^2)} = \mathcal{O}(\delta^{\tau_*}), \quad \delta \rightarrow 0. \quad (3.5)$$

for some $\tau_* > 0$, provided the slowly varying amplitudes $\alpha_j(\delta\mathbf{x}, \delta t)$, $j = 1, 2$ evolve according to the system of Dirac-type equations (3.6)-(3.7). Here, $\rho > 0$ and $\varepsilon_1 > 0$ are arbitrary.

In [6] we prove

Theorem 3.1. *Consider the time-dependent Schrödinger equation, (1.1), where $V(\mathbf{x})$ denotes a potential for which the conclusions of Theorem 2.1 hold, e.g. $V(\mathbf{x}) = \epsilon V_h(\mathbf{x})$, where V_h is a honeycomb lattice potential satisfying $V_{1,1} \neq 0$ and ϵ is not in the countable closed set $\tilde{\mathcal{C}}$. Let $\lambda_\sharp \in \mathbb{C}$, $\lambda_\sharp \neq 0$ be given by (2.8). Assume*

$$\vec{\alpha}_0(\mathbf{X}) \equiv \begin{pmatrix} \alpha_{10}(\mathbf{X}) \\ \alpha_{20}(\mathbf{X}) \end{pmatrix} \in [\mathcal{S}(\mathbb{R}^2)]^2$$

and let $\vec{\alpha}(\mathbf{X}, T)$ denote the global-in-time solution of the Dirac system

$$\partial_T \alpha_1(\mathbf{X}, T) = -\bar{\lambda}_\sharp (\partial_{X_1} + i\partial_{X_2}) \alpha_2(\mathbf{X}, T) \quad (3.6)$$

$$\partial_T \alpha_2(\mathbf{X}, T) = -\lambda_\sharp (\partial_{X_1} - i\partial_{X_2}) \alpha_1(\mathbf{X}, T). \quad (3.7)$$

with initial data $\vec{\alpha}(\mathbf{X}, 0) = \vec{\alpha}_0(\mathbf{X})$ and initial conditions, ψ_0 , of the form (3.2).

Fix any $\rho > 0, \varepsilon_1 > 0$ and $s \geq 1$. Then, (1.1) has a unique solution of the form (3.3), where for any $|\alpha| \leq N$

$$\sup_{0 \leq t \leq \rho \delta^{-2+\varepsilon_1}} \|\eta^\delta(\cdot, t)\|_{H^s(\mathbb{R}^2)} = o(\delta^{\tau_*}), \quad \delta \rightarrow 0 \quad (3.8)$$

for some $\tau_* > 0$.

Remark 3.1. In connection with Remark 2.2, we also consider the analogous question of the dynamics of solutions for wave-packet initial data, spectrally concentrated at a Dirac point of the deformed honeycomb structure. In this case, the large, but finite, time dynamics are given by *tilted*- Dirac equations. The latter can be mapped to the standard 2D Dirac equations by a Galilean change of variables.

Remarks on the proof of Theorem 3.1: We seek a solution of the initial value problem with wave-packet initial condition (3.2) of the form (3.3), a slow space/time modulation of the degenerate subspace plus an error term $\eta^\delta(x, t)$. The Dirac equations (3.6)-(3.7) arise as a non-resonance condition, which ensures that $\eta^\delta(\mathbf{x}, t)$ is small on a time interval: $0 \leq t \leq \mathcal{O}(\delta^{-2+})$. Estimation of η^δ , via its DuHamel integral equation, requires a careful decomposition of the propagator, $e^{-i(-\Delta+V)t}$ and analysis of its action on functions with quasi-momentum components supported near \mathbf{K}_* , a vertex of \mathcal{B} , and those with quasi-momentum components supported away from \mathbf{K}_* . The resonant terms, which are removed by imposing equations (3.6)-(3.7), arise from quasi-momenta near \mathbf{K}_* . A detailed expansion of the normalized Floquet-Bloch modes for such quasi-momenta is required. Such modes are discontinuous at \mathbf{K}_* . Components corresponding to quasi-momenta away from \mathbf{K}_* are controlled via Poisson summation and integration by parts with respect to time by making use of rapid phase oscillations in time.

Formal derivations of Dirac-type dynamics for honeycomb lattice structures are discussed in the physics [13] and applied mathematics [2] literature. A rigorous discussion of the tight-binding limit is presented in [1]. Conical singularities have long been known to occur in Maxwell equations with constant anisotropic dielectric tensor; see, for example, [10], [4] and references cited therein.

4. NLS / GP and the nonlinear Dirac equation

A model of fundamental importance in the description of macroscopic quantum phenomena and nonlinear optical phenomena is the *nonlinear Schrödinger / Gross-Pitaevskii equation*, (NLS/GP):

$$i\partial_t\psi = (-\Delta + V(\mathbf{x}))\psi + g|\psi|^2\psi \quad (4.1)$$

We refer to the case $V \equiv 0$ as the nonlinear Schrödinger equation (NLS). In the quantum setting, the potential, $V(\mathbf{x})$, models a magnetic trap confining a large number of quantum particles (bosons). A wide range of potentials, so called optical lattices, can be induced optically via interference of optical beams. We consider the case where $V = V_h$ is a honeycomb lattice potential in the sense of Definition 1.1. Analogously, in the setting of nonlinear electromagnetics interference of beams in photorefractive crystals can generate a spatially dependent index of refraction, corresponding to a honeycomb lattice potential. See, for example, [16, 5, 12, 3].

Our goal in this section is to give a formal derivation of a nonlinear Dirac equation from the NLS/GP and to pose some interesting questions to consider going forward.

We assume wave-packet initial conditions for NLS/GP, with amplitude scaled so that nonlinear effects and the Dirac dynamics enter on the same time-scale:

$$\psi^\delta(\mathbf{x}, t) = \left(\delta^{\frac{1}{2}} \sum_{j=1}^2 \alpha_j(\mathbf{X}, T) \Phi_j(\mathbf{x}) + \eta^\delta(\mathbf{x}, t) \right) e^{-i\mu_\star t}, \quad (4.2)$$

where $\mathbf{X} = \delta\mathbf{x}$ and $T = \delta t$. Substitution of the Ansatz (4.2) into NLS/GP, (4.1), yields $\eta^\delta = \delta^{\frac{1}{2}} (\delta\eta_1 + \mathcal{O}(\delta^2))$, where η_1 , satisfies:

$$\begin{aligned} & i\partial_t \eta_1(\mathbf{x}, t) - (H - \mu_\star) \eta_1(\mathbf{x}, t) \\ &= - \sum_{j=1}^2 \left(i\partial_T \alpha_j \Phi_j(\mathbf{x}) + 2\nabla_{\mathbf{x}} \alpha_j \cdot \nabla_{\mathbf{x}} \Phi_j(\mathbf{x}) - g \sum_{1 \leq i, l \leq 2} \alpha_i \alpha_j \bar{\alpha}_l \Phi_i(\mathbf{x}) \Phi_j(\mathbf{x}) \bar{\Phi}_l(\mathbf{x}) \right). \end{aligned} \quad (4.3)$$

A calculation which is analogous to that carried out and rigorously justified in [6] for the linear Schrödinger equation (see section 3) yields the following semilinear Dirac system governing the slowly modulating amplitudes $\alpha_1(\mathbf{X}, T)$ and $\alpha_2(\mathbf{X}, T)$:

$$\partial_T \alpha_1 = -\bar{\lambda}_\# (\partial_{X_1} + i\partial_{X_2}) \alpha_2 - i g (\beta_1 |\alpha_1|^2 + 2\beta_2 |\alpha_2|^2) \alpha_1, \quad (4.4)$$

$$\partial_T \alpha_2 = -\lambda_\# (\partial_{X_1} - i\partial_{X_2}) \alpha_1 - i g (2\beta_2 |\alpha_1|^2 + \beta_1 |\alpha_2|^2) \alpha_2. \quad (4.5)$$

The coefficients β_1 and β_2 are given in terms of the Floquet-Bloch modes:

$$\beta_1 = \int_{\Omega} |\Phi_1(\mathbf{x})|^4 d\mathbf{x} = \int_{\Omega} |\Phi_2(\mathbf{x})|^4 d\mathbf{x} \quad \text{and} \quad \beta_2 = \int_{\Omega} |\Phi_1(\mathbf{x})|^2 |\Phi_2(\mathbf{x})|^2 d\mathbf{x}. \quad (4.6)$$

The system (4.4)-(4.5) has the following conserved integrals:

$$\mathcal{N}[\alpha_1, \alpha_2] \equiv \int_{\mathbb{R}^2} (|\alpha_1|^2 + |\alpha_2|^2) dX_1 dX_2, \quad (4.7)$$

$$\begin{aligned} \mathcal{H}[\alpha_1, \alpha_2] &\equiv \text{Im} \left[\bar{\lambda}_\# \int_{\mathbb{R}^2} \alpha_2 (\partial_{X_1} + i\partial_{X_2}) \bar{\alpha}_1 dX_1 dX_2 \right] \\ &\quad - \frac{g}{4} \int_{\mathbb{R}^2} (\beta_1 |\alpha_1|^4 + 4\beta_2 |\alpha_1|^2 |\alpha_2|^2 + \beta_1 |\alpha_2|^4) dX_1 dX_2. \end{aligned} \quad (4.8)$$

A word about the calculation leading to (4.4)-(4.5): Heuristically speaking, the modulation equations (4.4)-(4.5) for $\alpha_j(\mathbf{X}, T)$, $j = 1, 2$, are obtained by choosing their slow, (\mathbf{X}, T) , evolution to cancel all resonant components of the forcing term in (4.3). This can be implemented by setting the projection of the forcing term onto the modes Φ_j , $j = 1, 2$ (integrating only over the fast variable, \mathbf{x}) to zero.

In computing this projection, many cubic terms drop by symmetry considerations. For example, consider the contribution of the cubic term: $\alpha_1 \alpha_1 \bar{\alpha}_2 \Phi_1 \Phi_1 \bar{\Phi}_2$ in (4.3) to the equation for α_1 . To compute this contribution take the $L^2(\mathbb{R}_{\mathbf{x}}^2)$ inner product

with $\Phi_1(\mathbf{x})$:

$$\begin{aligned}
\langle \Phi_1, \Phi_1 \Phi_1 \overline{\Phi_2} \rangle_{L^2(\Omega)} &= \int_{\Omega} \overline{\Phi_1(\mathbf{x})} \cdot \Phi_1(\mathbf{x}) \Phi_1(\mathbf{x}) \overline{\Phi_2(\mathbf{x})} \, d\mathbf{x} \\
&=_{\mathbf{x}=R^*\mathbf{y}} \int_{R\Omega} \overline{\Phi_1(R^*\mathbf{y})} \cdot \Phi_1(R^*\mathbf{y}) \Phi_1(R^*\mathbf{y}) \overline{\Phi_2(R^*\mathbf{y})} \, d\mathbf{y} \\
&= \int_{R\Omega} \overline{\tau \Phi_1(\mathbf{y})} \cdot \tau \Phi_1(\mathbf{y}) \cdot \tau \Phi_1(\mathbf{y}) \cdot \overline{\tau \Phi_2(\mathbf{y})} \, d\mathbf{y} \\
&= \tau^2 \int_{\Omega} \overline{\Phi_1(\mathbf{x})} \cdot \Phi_1(\mathbf{x}) \Phi_1(\mathbf{x}) \overline{\Phi_2(\mathbf{x})} \, d\mathbf{x} = \tau^2 \langle \Phi_1, \Phi_1 \Phi_1 \overline{\Phi_2} \rangle_{L^2(\Omega)}
\end{aligned}$$

Therefore,

$$(1 - \tau^2) \langle \Phi_1, \Phi_1 \Phi_1 \overline{\Phi_2} \rangle_{L^2(\Omega)} = 0 \implies \langle \Phi_1, \Phi_1 \Phi_1 \overline{\Phi_2} \rangle_{L^2(\Omega)} = 0.$$

It follows that a term of the form $\alpha_1 \overline{\alpha_2} \alpha_1$ does not appear in the (4.4).

An alternative formal approach to obtaining (4.4)-(4.5) is by the method of multiple scales; see [2] where a formal derivation of a semilinear Dirac system for a small (“shallow”) honeycomb lattice potential of a special form is presented and studied numerically.

As in the proof of Theorem 3.1, a proof of the large time validity of the nonlinear Dirac system (4.4)-(4.5) requires establishing that η^δ remains small in a suitable norm on a large (growing as $\delta \downarrow 0$) time scale. This rests on a study of the time-evolution of the Floquet-Bloch components of η^δ which are near \mathbf{K}_* and away from \mathbf{K}_* , together with an understanding of bounds on the solutions to the nonlinear Dirac equations (4.4)-(4.5).

We conclude with some natural questions. Is there global well-posedness for the initial value problem for semi-linear Dirac system (4.4)-(4.5) or do solutions develop singularities (blow up) in finite time? How do the corresponding solutions of NLS / GP behave?

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