On Tight-Binding Approximations in Optical Lattices

By Mark J. Ablowitz, Christopher W. Curtis, and Yi Zhu

The validity of using the tight-binding approximation for the nonlinear Schrödinger equations with a two-dimensional optical lattice is considered. This work provides a rigorous foundation for a technique based on "orbital" functions that is central to solid-state physics and nonlinear optics. Simple and honeycomb lattices are addressed, and it is therefore shown that the use of tight-binding approximations is justified in complicated situations.

1. Introduction

Many interesting advances in nonlinear optics in recent years have come from studying a laser beam impinging upon a periodic lattice. These lattices are two-dimensional realizations of the now classic one-dimensional dielectric materials with transversely varying index of refraction, cf. [1]. Similar lattice problems were considered many years ago in solid-state physics where atoms are arranged in a lattice (cf. [2], [3], [4]) and then in Bose-Einstein condensates (BECs) where cold atoms are trapped in an optically induced lattice, cf. [5]. The standard model of a field interacting with a lattice is the nonlinear Schrödinger equations with an additional potential (also called the Gross-Pitaevskii equation in BECs)

$$iu_z + \Delta u - \frac{1}{h^2} V(\mathbf{r})u + \sigma |u|^2 u = 0, \tag{1}$$

with $V(\mathbf{r}) \in C^\infty(\mathbb{R}^2)$, $V(\mathbf{r} + \mathbf{v}_j) = V(\mathbf{r})$ for $1 \leq j \leq 2$, $V \geq 0$, and h and σ real constants.

Address for correspondence: Christopher W. Curtis, Department of Applied Mathematics, University of Colorado, Boulder, CO 80309, USA; e-mail: christopher.w.curtis@colorado.edu

DOI: 10.1111/j.1467-9590.2012.00558.x
STUDIES IN APPLIED MATHEMATICS 129:362–388

In nonlinear optics, this equation describes electromagnetic waves propagating in inhomogeneous, Kerr nonlinear media. The equation can be derived from the Maxwell equations by assuming a unidirectionally polarized field and the paraxial approximation; here z is the propagation direction, $V(\mathbf{r})$ represents the spatial variation of the linear refractive index, and σ is the coefficient which is positive for focusing or negative for defocusing nonlinearity. In BECs, it describes the dynamics of a macroscopic quantum state of ultracold atoms being trapped in an optical lattice in the mean-field limit. The nonlinearity is due to two-particle interactions and the nonlinear coefficient σ corresponds to the scattering length, cf. [5].

Fully describing the wave dynamics in Equation (1) is both analytically and computationally complex. Therefore, homogenized equations were derived to analyze the dynamics of specific wave envelopes . This reduction is under the assumption that the envelope scale is much larger than the lattice scale. On the other hand, a discrete approach was introduced without assuming the large envelope scale. This approach is valid in the sense of the tight-binding limit, i.e., $0 < h \ll 1$, where one assumes that the potential has localized minima, and the relative depth of these minima compared to nearby maxima is very large. Then one can model this system as though the local minima are independent. In this way, one can generate wave-functions, called orbitals in this paper, associated with each minima and then model the full dynamics associated with the original potential by taking appropriately weighted linear combinations of the orbitals. When appropriate, the tight-binding approximation provides a simple means of generating approximations to (1). This approximation technique forms the basis of the papers [6] and [7], the results of which we rigorously establish here.

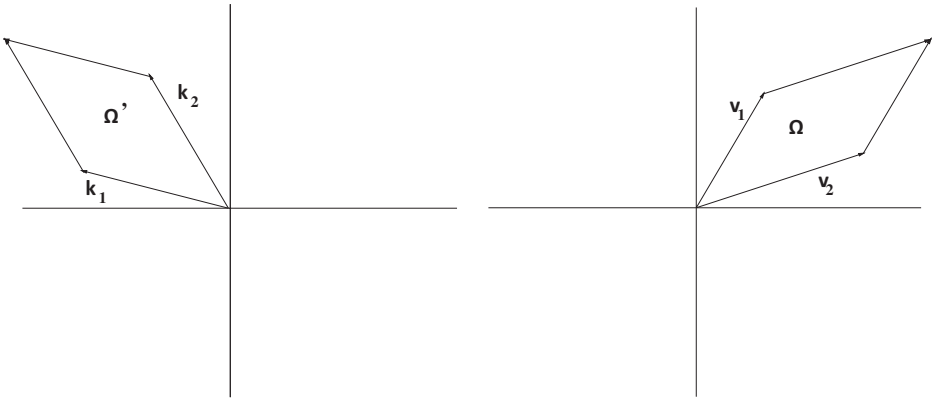
In order to elaborate on the tight-binding approximation, we first introduce some notation and assumptions. Using the period vectors $\mathbf{v}_1$ and $\mathbf{v}_2$, we generate a lattice $\mathcal{P}$ where

$$\mathcal{P} = \left\{ \sum_{j=1}^{2} m_j \mathbf{v}_j : m_j \in \mathbb{Z} \right\}.$$

As a point of reference, we place $\mathbf{v}_1$ and $\mathbf{v}_2$ at the origin and define the primitive cell Ω to be the cell formed by these lattice vectors. Likewise, we define the dual lattice, or Brillouin zone, $\mathcal{G}$ as the lattice formed by the vectors $\mathbf{k}_j$ such that $\mathbf{k}_j \cdot \mathbf{v}_l = 2\pi\delta_{jl}$, cf. [8]. We also define the dual primitive cell, Ω', with $\mathbf{k}_1$ and $\mathbf{k}_2$ located at the origin; see Figure 1. We also assume that $\max |V| = 1$, and V can take on only isolated minima at its zeros, which are called wells.

Given the above assumptions on the lattice, and defining the operator

$$L_h = -\Delta + \frac{1}{h^2} V,$$



(a) Dual Lattice (b) Periodic Lattice

Figure 1. Dual lattice (left) and lattice (right).

the core of building tight-binding approximations to solutions of (1) is an understanding of the spectrum, $\sigma(L_h)$, of L_h. Thus, we present the following basic facts that are used throughout the paper. Following [9] and [8], one has in $L^2(\mathbb{R}^2)$ that $\sigma(L_h)$ is absolutely continuous and can be written as

$$\sigma(L_h) = \bigcup_{\mathbf{k}} \sigma(L_{h,\mathbf{k}}),$$

where $L_{h,\mathbf{k}}$ is posed on $L^2(\Omega)$ and is given by

$$L_{h,\mathbf{k}} = -\Delta - 2i\mathbf{k}\cdot\nabla + |\mathbf{k}|^2 + \frac{1}{h^2}V(\mathbf{r})$$

with $\mathbf{k}$ taking on all values in Ω'. The operator $L_{h,\mathbf{k}}$ has a compact resolvent, and therefore $\sigma(L_{h,\mathbf{k}})$ is discrete, being composed of some countable number of $\mathbf{k}$ dependent eigenvalues, $\mu_l(\mathbf{k})$, so that we may write

$$\sigma(L_{h,\mathbf{k}}) = \bigcup_{l\geq 0} \mu_l(\mathbf{k}).$$

We define the lth band, B_l of $\sigma(L_h)$, as

$$B_l = \bigcup_{\mathbf{k}\in\Omega'} \mu_l(\mathbf{k}),$$

so that one can write $\sigma(L_h)$ as

$$\sigma(L_h) = \bigcup_{l\geq 0} B_l.$$

Note, since $L_{h,\mathbf{k}}$ is self adjoint, B_l consists of only real values. Likewise, one can think of the dispersion relationships $\mu_l(\mathbf{k})$ as continuous maps over a compact domain, and thus the bands B_l are closed. Associated with the eigenvalue, or dispersion relationship, $\mu_l(\mathbf{k})$, one defines the Bloch-mode $\varphi_l(\mathbf{r}, \mathbf{k})$ by

$$L_h\varphi_l = \mu_l(\mathbf{k})\varphi_l, \tag{2}$$

which implies $\varphi_l(\mathbf{r} + \mathbf{v}_j, \mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{v}_j}\varphi_l(\mathbf{r}, \mathbf{k})$ and $\varphi_l(\mathbf{r}, \mathbf{k} + \mathbf{k}_j) = \varphi_l(\mathbf{r}, \mathbf{k})$ for all j. Likewise $\mu_l(\mathbf{k} + \mathbf{k}_j) = \mu_l(\mathbf{k})$ for $1 \le j \le 2$.

We can now further elaborate on the tight-binding approximation that was used to approximate solutions of (1) in [6], where potentials with only one well per lattice cell, or simple lattices, were examined, and [7], where potentials with two wells per lattice cell, or non-simple honeycomb (HC) lattices, were studied. Note, the approach used in these papers builds upon the work in [10], [11], [12], [13], [14], and [15]. In the case of simple lattices, the tight-binding approximation begins with defining an orbital function ϕ, which is the ground-state eigenvector of the Schrödinger equations

$$-\Delta + \frac{1}{h^2}V_{orb},$$

where $V_{orb} = V + \tilde{\delta}V_{orb}$. The choice of $\tilde{\delta}V_{orb}$ is described later in the text, but the key component in its construction is that it forces V_{orb} to have an isolated global minimum. The authors of [6] and [7] then choose the initial condition for (1)

$$u(\mathbf{r}, 0) = \sqrt{\frac{\epsilon}{g}}\sum_{\mathbf{v}} a_{\mathbf{v},0}\phi(\mathbf{r} - \mathbf{v}), \tag{3}$$

where $\mathbf{v}$ denotes a vector in the lattice formed by $\mathbf{v}_1$ and $\mathbf{v}_2$, $g = ||\phi||^4_{L^4(\mathbb{R}^2)}$, $\sum_{\mathbf{v}} |a_{\mathbf{v},0}| < \infty$, and ϵ is a small parameter that vanishes as $h \to 0$. Multiple-scale arguments are presented in [7] that show the dominant behavior of the solution to (1) for the given initial condition is given by

$$u_{apx}(\mathbf{r}, z) = \sqrt{\frac{\epsilon}{g}}\left(\sum_{\mathbf{v}} a_{\mathbf{v}}(\epsilon z)\phi(\mathbf{r} - \mathbf{v})\right)e^{-i\mu_0(\mathbf{k})z}, \tag{4}$$

where $a_{\mathbf{v}}(0) = a_{\mathbf{v},0}$. Note: in [6] and [7], there is added $\mathbf{k}$ dependence of the form $a_{\mathbf{v}} = a_{\mathbf{v}}(\epsilon z, \mathbf{k}) = \tilde{a}_{\mathbf{v}}e^{i\mathbf{k}\cdot\mathbf{v}}$. In this paper, the coefficients depend on $\mathbf{k}$ in the same way, so that $|a_{\mathbf{v}}| = |\tilde{a}_{\mathbf{v}}|$. With the $\mathbf{k}$ dependence, the continuum limit of the discrete system describing the evolution of the coefficients $a_{\mathbf{v}}$ is shown to be a NLS equation whose dispersive term depends on the Hessian of $\mu_0(\mathbf{k})$ (cf. [6], [7]). We suppress this additional $\mathbf{k}$ dependence for simplicity of representation, though the results presented do not change if one allows the coefficients to vary in $\mathbf{k}$. The major results in [6] and [7] are the derivations of discrete nonlinear systems; in [6], a discrete nonlinear Schrödinger (DNLS) equations

determines the dynamics of the coefficients $a_{\mathbf{v}}(\epsilon z)$. The DNLS equation is given in Section 3 by Equation (9). In [7], the above method was generalized to non-simple HC lattices to yield a discrete Dirac system for a general value of $\mathbf{k}$ in the Brillouin zone; this is given in Section 5 by Equation (18). More details on these discrete systems are provided later in the text.

Since the work in [6] and [7] was formal, it is desirable to provide additional mathematical support. Thus in this paper, we provide rigorous justification of the validity of the tight-binding approximation in the case of a simple lattice, and we also outline how to do this for the non-simple HC lattice case.

To show our results, we use the following spaces.

- The sth Sobolev space $H_s(\mathbb{R}^2)$ is denoted by

$$||f||^2_{H_s(\mathbb{R}^2)} = \int_{\mathbb{R}^2} (1 + |\xi|^2)^s |\mathcal{F}(f)|^2 d\xi,$$

  where $\mathcal{F}(\cdot)$ denotes the Fourier transform. Note, $L^2(\mathbb{R}^2) = H_0(\mathbb{R}^2)$.
- We define the space $l^2_s(\mathcal{P})$ as those sequences $a_{\mathbf{p}}$, $\mathbf{p} \in \mathcal{P}$, such that

$$||a||^2_{l^2_s(\mathcal{P})} = \sum_{\mathbf{p}} (1 + |\mathbf{p}|^2)^s |a_{\mathbf{p}}|^2 < \infty.$$

  Likewise we define $l^1(\mathcal{P})$ via the norm

$$||a||_{l^1(\mathcal{P})} = \sum_{\mathbf{p}} |a_{\mathbf{p}}|.$$

Then we prove the following theorem:

THEOREM 1. *Define*

$$\epsilon = \frac{e^{-\tilde{b}/h}}{h^4},$$

where $\tilde{b} > 0$, *and choose coefficients* $a_{\mathbf{v},0}$ *in* (3) *such that* $\{a_{\mathbf{v},0}\} \in l^2_s$, $s > 1$. *Then, for a simple lattice, using initial condition* (3), *for* h *sufficiently small, there exists a solution to (1),* $u(\mathbf{r}, z)$, *such that*

$$||u(\mathbf{r}, z) - u_{apx}(\mathbf{r}, z)||_{H_2(\mathbb{R}^2)} = \mathcal{O}(\epsilon^{\frac{1}{2}+\alpha}),$$

where u_{apx} *is given by* (4) *and* $\{a_{\mathbf{v}}\}$ *solves* (9), *for values* z *such that* $z = \mathcal{O}(\epsilon^{-1+\alpha})$, *where* $0 < \alpha < 1$.

Modulo a few technical details that are omitted for clarity and ease of reading, this result holds for non-simple HC lattices as well, and the analogous result is presented in Section 5. In Section 2, we describe the orbital approximation for simple lattices. Section 3 introduces the discrete system for simple lattices, and Section 4 presents our proof of Theorem 1. Section 5 presents a summary

of the relevant information concerning non-simple HC lattices, and we provide a brief summary of how to extend Theorem 1 and then state the relevant theorem. Section 6 shows how to approximate orbitals by radially symmetric functions; this employs the WKB method with a turning point at the origin and homogeneous Dirichlet boundary conditions. This section gives a concrete way to approximate all of the relevant quantities used throughout the paper.

Previous work on the rigorous justification of tight-binding approximations using so-called Wannier functions have appeared, cf. [16] and [17]. The authors of [16] and [17] were able to get, in the H_1 norm, $\mathcal{O}(\epsilon^{3/2})$ error on z-scales of $\mathcal{O}(\epsilon^{-1})$. However, this was done by focusing on one-dimensional, piecewise constant potentials that allow for explicit computations. We are not able to perform such explicit computations since we treat much more general, two-dimensional potentials. Another major difference is that here we use orbitals, not Wannier functions, where the Wannier function associated with the lowest band $\mu_0(\mathbf{k})$, $\hat{\varphi}_{0,0}$, is defined by

$$\hat{\varphi}_{0,0}(\mathbf{r}) = \int_{\Omega'} \varphi_0(\mathbf{r}, \mathbf{k}) d\mathbf{k}. \tag{5}$$

The Wannier functions possess nice analytic properties that in some cases make working with them useful. However, for non-simple HC lattices where the first two bands are exponentially close, getting pointwise estimates of Wannier functions is difficult (cf. [18] and [19] for further discussion on this point). However we find the use of orbitals enjoys an advantage over the Wannier functions in that orbitals allow for the ready use of standard asymptotic methods such as WKB to obtain estimates of the parameters used in the tight-binding approximation. Hence the orbital approach is a practical means by which to approximate solutions to (1). Indeed the orbital approach has been used extensively in the physics literature for over 70 years (cf. [2], [3], [4]). Another distinguishing feature between using orbitals and Wannier functions appears in the non-simple HC lattice case. Since Wannier functions, as seen in (5), are defined on the entire lattice cell, it is neither clear nor straightforward how to use them to study interactions between wells within a cell.

2. The orbital approximation

In what follows, we assume that our potential has forms a simple lattice and has a single well at the origin within the primitive cell Ω such that $V(0) = 0$, $\nabla V(0) = 0$, and

$$V(\mathbf{r}) = \frac{1}{2}\mathbf{r}^T V''(0)\mathbf{r} + o(\mathbf{r}), \text{ as} |\mathbf{r}| \to 0,$$

where $V''(0)$ is the Hessian of V at the origin, and $\mathbf{r}^T$ is the transpose of the vector $\mathbf{r}$. Further, if $\mathbf{r} \neq 0$ then $V(\mathbf{r}) > 0$. Thus the well represents the global minima on the primitive cell Ω. We now introduce one of the key analytic ingredients necessary for establishing rigorous results on tight binding, the Agmon metric. Given our assumptions on V, following [20], define the Agmon metric, $d_A(\mathbf{r}, \mathbf{r}')$, as

$$d_A(\mathbf{r}, \mathbf{r}') = \inf_{\gamma} \int_0^1 \sqrt{V(\gamma(t))} |\dot{\gamma}(t)| dt,$$

where $\gamma(t)$ is an absolutely continuous curve such that $\gamma(0) = \mathbf{r}$ and $\gamma(1) = \mathbf{r}'$. As shown in [20] and elsewhere, the Agmon metric satisfies the triangle inequality, is locally Lipschitz continuous in each variable, and is symmetric, i.e., $d_A(\mathbf{r}, \mathbf{r}') = d_A(\mathbf{r}', \mathbf{r})$. Generally, the Agmon metric can be degenerate, i.e., $d(\mathbf{r}, \mathbf{r}') = 0$ does not imply $\mathbf{r} = \mathbf{r}'$. However, we can show the following lemma:

LEMMA 1. *Given that the potential V has isolated minima or wells, the Agmon metric is nondegenerate.*

Proof: We wish to show that $d_A(\mathbf{r}, \mathbf{r}') = 0$ if and only if $\mathbf{r} = \mathbf{r}'$. First suppose that either $\mathbf{r}$ or $\mathbf{r}'$ is not a well. Since the Agmon metric is symmetric, without loss of generality we assume $\mathbf{r}'$ is not a well. Thus, there is some ball of radius ϵ, $B(\mathbf{r}', \epsilon)$, such that $V > c_\epsilon^2$ within the ball. Thus along any path $\gamma(t)$ such that $\gamma(1) = \mathbf{r}'$, there must be some t^* such that $\gamma(t)$ is within $B(\mathbf{r}', \epsilon)$ for $t^* \leq t \leq 1$ and $|\mathbf{r}' - \gamma(t^*)| = \epsilon$. Therefore for any absolutely continuous curve $\gamma(t)$, we have

$$\begin{aligned}
\int_0^1 \sqrt{V(\gamma(t))} |\dot{\gamma}(t)| dt &= \int_0^{t^*} \sqrt{V(\gamma(t))} |\dot{\gamma}(t)| dt + \int_{t^*}^1 \sqrt{V(\gamma(t))} |\dot{\gamma}(t)| dt \\
&\geq c_\epsilon \int_{t^*}^1 |\dot{\gamma}(t)| dt \\
&\geq c_\epsilon |\mathbf{r}' - \gamma(t^*)|,
\end{aligned}$$

where the last inequality comes from the fact that the shortest path between two points in the plane is a straight line. Thus in this case $d(\mathbf{r}, \mathbf{r}') \geq c_\epsilon \epsilon$.

Hence the result holds if $\mathbf{r}$ and $\mathbf{r}'$ are not both wells. If both are wells, then this means that there is at least one point along any path between the wells such that a neighborhood around this point does not contain a well. Thus repeating the argument from above about this point establishes the result. ■

Now define the constant S_0 such that

$$S_0 = \inf_{\mathbf{v} \neq 0} d_A(0, \mathbf{v}),$$

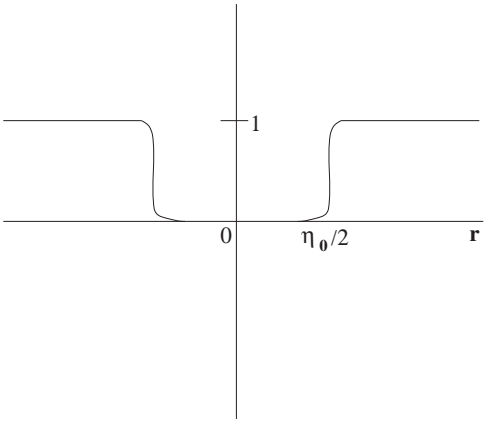


Figure 2. $1 - \chi(\mathbf{r})$.

where $\mathbf{v} \in \mathcal{P}$ is a lattice vector. Then, define the ball $B_A(0, S)$ as

$$B_A(0, S) = \{\mathbf{r} \in \mathbb{R}^2 : d_A(0, \mathbf{r}) < S\}.$$

Choosing some value $\eta_0 < S_0$, we define the function χ to be smooth, satisfy $0 \leq \chi \leq 1$, have compact support in $B_A(0, \eta_0)$, and $\chi|_{B_A(0, \frac{\eta_0}{2})} = 1$.

We define the potential

$$V_{orb} = V + (1 - \chi),$$

and we likewise define

$$\tilde{\delta} V_{orb} = V_{orb} - V = 1 - \chi.$$

See Figure 2 for a profile of $1 - \chi(\mathbf{r})$.

By construction, V_{orb} is a one-well potential, and therefore a number of theorems become available to us when we solve the eigenvalue problem

$$-\Delta\phi + \frac{1}{h^2} V_{orb}(\mathbf{r})\phi = \tilde{E}_0\phi \tag{6}$$

for $\phi \in L^2(\mathbb{R}^2)$. Since $V''(0) > 0$, we let $V''(0) = \tilde{U}^{-1}\Lambda\tilde{U}$, and let $\mathbf{y} = \tilde{U}\mathbf{r}$ where $\tilde{U}$ is unitary and D is diagonal since $V''(0)$ is self-adjoint. We define the harmonic oscillator problem

$$-\Delta_{\mathbf{y}}\psi + \mathbf{y}^T\Lambda\mathbf{y}\psi = E_0\psi, \tag{7}$$

with $E_0 = \sqrt{\Lambda_1} + \sqrt{\Lambda_2}$, where Λ_j are the nonzero entries in the diagonal matrix Λ. We then have the following three theorems:

THEOREM 2. [21] *The lowest eigenvalue* $\tilde{E}_0$ *in* (6) *is simple and has the expansion*

$$\tilde{E}_0 = \frac{E_0}{h} + \mathcal{O}(h^{-1/2}),$$

where E_0 *is defined in (7).*

THEOREM 3. [22] *The following asymptotic expansion*

$$\mu_0(\mathbf{k}) = \tilde{E}_0 + \mathcal{O}\left(\frac{e^{-(S_0-\eta_0)/h}}{h^2}\right),$$

holds uniformly for all $\mathbf{k} \in \Omega'$ *with* S_0 *and* η_0 *defined above.*

THEOREM 4. [21] *For any* $0 < \delta < 1$*, there exists a constant* $C_\delta > 0$ *such that*

$$||e^{(1-\delta)d_A(x,0)/h}\phi||_{H_1(\mathbb{R}^2)} \leq C_\delta e^{\delta/h}.$$

Note, Theorem 4 shows in principle that the eigenfunction ϕ decays exponentially fast which is a very useful fact as is shown later.

Let $\phi_{\mathbf{p}}(\mathbf{r}) = \phi(\mathbf{r} - \mathbf{p})$. With these definitions and the previous theorems, we now prove the following lemma:

LEMMA 2. *There exists a constant* $\tilde{b} > 0$ *such that, for* $\mathbf{p} \neq 0$,

$$\begin{aligned} < \phi, \phi_{\mathbf{p}} > &= \mathcal{O}(e^{-\tilde{b}/h}), \\ < \tilde{\delta} V_{orb}\phi, \phi_{\mathbf{p}} > &= \mathcal{O}(e^{-\tilde{b}/h}), \\ < \tilde{\delta} V_{orb}\phi, \phi > &= \mathcal{O}(e^{-2\tilde{b}/h}), \\ ||\tilde{\delta} V_{orb}\phi||_2 &= \mathcal{O}(e^{-\tilde{b}/h}). \end{aligned}$$

Proof: We start with, where $\mathbf{p} \neq 0$,

$$< \phi_{\mathbf{p}}, \phi >= \int_{\mathbb{R}^2} \phi(\mathbf{r} - \mathbf{p})\phi(\mathbf{r})d\mathbf{r}.$$

We then write

$$\int_{\mathbb{R}^2} = \int_{B_A(0)} + \int_{B_A(\mathbf{p})} + \int_{\mathbb{R}^2 \setminus (B_A(0) \cup B_A(\mathbf{p}))},$$

where $B_A(\mathbf{p})$ is short for $B_A(\mathbf{p}, \frac{\eta_0}{2})$. See Figure 3 for more detail. Using

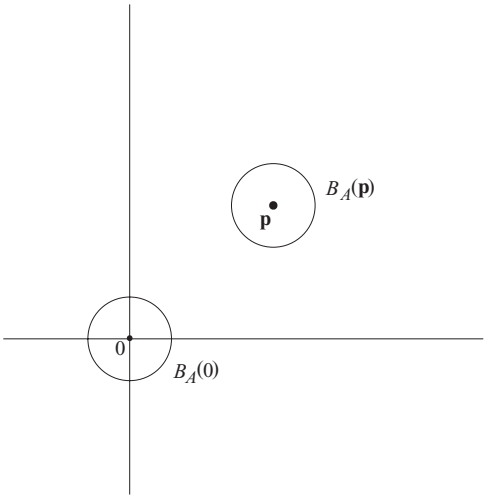


Figure 3. Domain decomposition.

Theorem 3 and the Cauchy-Schwarz inequality, we have

$$\left|\int_{B_A(0)} \phi(\mathbf{r}-\mathbf{p})\phi(\mathbf{r})d\mathbf{r}\right| \leq \int_{B_A(0)} e^{-(1-\delta)d_A(\mathbf{r}-\mathbf{p},0)/h} \left|\phi_{\mathbf{p}}\right| e^{(1-\delta)d_A(\mathbf{r}-\mathbf{p},0)/h} |\phi|\, d\mathbf{r}$$

$$\leq C_\delta e^{-((1-\delta)b_0-\delta)/h},$$

where the constant b_0 is defined by

$$b_0 = \inf_{\mathbf{p}\neq 0} \inf_{\mathbf{r}\in B_A(0)} d_A(\mathbf{r}-\mathbf{p}, 0),$$

which must be positive given the non-degeneracy of the Agmon metric as shown in Lemma 1.

Repeating our argument, we show that

$$\left|\int_{B_A(\mathbf{p})} \phi_{\mathbf{p}}\phi\right| \leq C_\delta e^{-((1-\delta)b_1-\delta)/h},$$

with

$$b_1 = \inf_{\mathbf{p}\neq 0} \inf_{B_A(\mathbf{p})} d_A(\mathbf{r}, 0).$$

Finally, letting $W(\mathbf{p}) = \mathbb{R}^2\backslash(B_A(0) \cup B_A(\mathbf{p}))$, we have that

$$\left|\int_{W(\mathbf{p})} \phi(\mathbf{r}-\mathbf{p})\phi(\mathbf{r})d\mathbf{r}\right| \leq ||\phi||_{L^2(W(\mathbf{p}))}||\phi_{1,\mathbf{p}}||_{L^2(W(\mathbf{p}))}$$

$$\leq C_\delta^2 e^{-((1-\delta)(b_2+b_3)-2\delta)/h},$$

where

$$b_2 = \inf_{\mathbf{p}\neq 0} \inf_{W(\mathbf{p})} d_A(\mathbf{r}, 0)$$

and

$$b_3 = \inf_{\mathbf{p}\neq 0} \inf_{W(\mathbf{p})} d_A(\mathbf{r} - \mathbf{p}, 0).$$

Thus choosing δ sufficiently small, we see we can make all three integrals exponentially small.

For the terms with the difference in potential, the analysis is essentially the same as above. We have that

$$| < \tilde{\delta} V_{orb}\phi, \phi > | \leq \int_{\mathbb{R}^2 \setminus B_A(0)} |\phi(\mathbf{r})|^2 \, d\mathbf{r},$$

$$\leq C_\delta^2 e^{-2((1-\delta)b_0 - \delta)/h}.$$

An identical argument establishes the same result for $||\tilde{\delta} V_{orb}\phi||_{L^2(\mathbb{R}^2)}$. Likewise, we can show that

$$| < \tilde{\delta} V_{orb}\phi, \phi_{\mathbf{p}} > | \leq \int_{\mathbb{R}^2 \setminus B_A(0)} |\phi(\mathbf{r})| \, |\phi(\mathbf{r} - \mathbf{p})| \, d\mathbf{r},$$

$$\leq C_\delta e^{-((1-\delta)b_1 - \delta)/h} + C_\delta^2 e^{-((1-\delta)(b_2+b_3) - 2\delta)/h}.$$

Thus, choosing δ such that $(1-\delta)b_0 - \delta > 0$, $(1-\delta)b_1 - \delta > 0$, and $(1-\delta)(b_2 + b_3) - 2\delta > 0$, take $\tilde{b}$ as the minimum of these three quantities. Thus the result is shown. ■

We now compare the two different scales that have so far appeared. Given that $\tilde{b}(\eta_0)$ tends to zero for $\eta_0 \to 0$ and $\eta_0 \to \infty$ (from the Cauchy-Schwartz inequality), but since $\tilde{b} > 0$ otherwise, then there is a value of η_0 such that $S_0 - \eta_0 = \tilde{b}$. Although we only need $S_0 - \eta_0 > \tilde{b}$, it is convenient to make them equal. We thus define the value ϵ as

$$\epsilon = \frac{e^{-\tilde{b}/h}}{h^4}.$$

This balance is useful in the proof of Theorem 1 (see Section 4). With ϵ now defined, it follows that

LEMMA 3. $\dfrac{1}{h^2} ||\tilde{\delta} V_{orb}\phi||_{H_2} = \mathcal{O}(\epsilon)$

Proof: Note, for any function f, we have

$$||f||_{H_2} = ||(-1 + \Delta)f||_2 \leq ||f||_2 + ||\Delta f||_2.$$

So establishing that $||\Delta(\tilde{\delta}V_{orb}\phi)||_2/h^2 = \mathcal{O}(\epsilon)$ proves the desired result since we have already established that $||\tilde{\delta}V_{orb}\phi||_2/h^2 = \mathcal{O}(\epsilon)$ in Lemma 2. Using the triangle inequality, we have

$$\begin{aligned}||\Delta(\tilde{\delta}V_{orb}\phi)||_2 &\leq ||\phi\Delta\tilde{\delta}V_{orb}||_2 + 2||\nabla\phi\cdot\nabla\tilde{\delta}V_{orb}||_2 + ||\tilde{\delta}V_{orb}\Delta\phi||_2\\ &\leq ||\phi\Delta\tilde{\delta}V_{orb}||_2 + 2||\nabla\phi\cdot\nabla\tilde{\delta}V_{orb}||_2\\ &\quad + \frac{1}{h^2}||\tilde{\delta}V_{orb}V_{orb}\phi||_2 + \tilde{E}_0||\tilde{\delta}V_{orb}\phi||_2.\end{aligned}$$

Since $\Delta\tilde{\delta}V_{orb}$ is zero on $B_A(0)$, then $||\phi\Delta\tilde{\delta}V_{orb}||_2/h^2 = \mathcal{O}(\epsilon)$. Likewise, using the fact that $\tilde{\delta}V_{orb}$ is zero on $B_A(0)$ gives that $||\tilde{\delta}V_{orb}V_{orb}\phi||_2/h^4$ and $\tilde{E}_0||\tilde{\delta}V_{orb}\phi||_2/h^2$ are both $\mathcal{O}(\epsilon)$. Finally, using the Cauchy-Schwarz inequality we have

$$|\nabla\phi\cdot\nabla\tilde{\delta}V_{orb}| \leq |\nabla\phi||\nabla\tilde{\delta}V_{orb}|,$$

where $|\cdot|$ denotes the Euclidean norm. The function $|\nabla\tilde{\delta}V_{orb}|$ is zero on $B_A(0)$, and therefore using Theorem 3, we have that $||\nabla\phi\cdot\nabla\tilde{\delta}V_{orb}||_2/h^2 = \mathcal{O}(\epsilon)$ using the same arguments as in Lemma 2. ■

Finally, we prove one more technical lemma that is used later in the paper.

LEMMA 4. *We have that* $||\phi||^{-4}_{L^4(\mathbb{R}^2)} = \mathcal{O}(1)$.

Proof: To prove the statement, we note that

$$||\phi||^4_{L^4(R^2)} = \int_{B_A(0)}|\phi|^4 d\mathbf{r} + \int_{\mathbb{R}^2\setminus B_A(0)}|\phi|^4 d\mathbf{r}.$$

Given this equality, using Hölder's (reverse) inequality, we have that $L^4(B_A(0)) \subset L^2(B_A(0))$, which implies that there is some constant $\tilde{c}$ such that

$$||\phi||^4_{L^4(\mathbb{R}^2)} \geq \tilde{c}\left(\int_{B_A(0)}|\phi|^2 d\mathbf{r}\right)^2 + \int_{\mathbb{R}^2\setminus B_A(0)}|\phi|^4 d\mathbf{r}.$$

The constant $\tilde{c}$ is independent of h, and clearly the second integral in the inequality is $\mathcal{O}(\epsilon)$. Likewise we have

$$\int_{B_A(0)}|\phi|^2 d\mathbf{r} = 1 + \mathcal{O}(\epsilon),$$

so that $||\phi||^4_{L^4(\mathbb{R}^2)} \geq \tilde{c} + \mathcal{O}(\epsilon)$, or

$$\frac{1}{||\phi||^4_{L^4(\mathbb{R}^2)}} = \mathcal{O}(1).$$

■

3. Derivation of the lattice equations

As stated before, we use a tight-binding approximation to solve the equation

$$i\psi_z - L_h\psi + \sigma|\psi|^2\psi = 0.$$

Therefore, we expand ψ into

$$\psi(\mathbf{r}, z) = \sqrt{\frac{\epsilon}{g}}\,(\phi_w(\mathbf{r}, \epsilon z) + \epsilon^\alpha R(\mathbf{r}, z))\, e^{-i\mu_0(\mathbf{k})z},$$

where $g = ||\phi||^4_{L^4(R^2)}$, and $0 < \alpha < 1$. Defining the slow scale $\tau = \epsilon z$, we substitute the above representation for ψ into the lattice nonlinear Schrödinger equations and find

$$\begin{aligned} i\epsilon\partial_\tau\phi_w + i\epsilon^\alpha R_z - (L_h - \mu_0(\mathbf{k}))\phi_w - \epsilon^\alpha(L_h - \mu_0(\mathbf{k}))R \\ + \frac{\sigma\epsilon}{g}|\phi_w + \epsilon^\alpha R|^2(\phi_w + \epsilon^\alpha R) = 0, \end{aligned} \tag{8}$$

where ϕ_w is written using the tight-binding approximation via orbitals as

$$\phi_w = \sum_{\mathbf{v}} a_{\mathbf{v}}(\tau)\phi_{\mathbf{v}}(\mathbf{r}).$$

Inserting this approximation then into (8) and taking the inner product with respect to $\phi_{\mathbf{p}}$ and dropping R, one gets the following discrete system [6]:

$$i\epsilon\frac{da_{\mathbf{p}}}{d\tau} + (\mu_0(\mathbf{k}) - \tilde{E}_0)a_{\mathbf{p}} - \sum_{<0>} a_{\mathbf{p}+\mathbf{v}}\lambda_{\mathbf{v}} + \epsilon\sigma|a_{\mathbf{p}}|^2 a_{\mathbf{p}} = 0, \tag{9}$$

where $\mathbf{p} \in \mathcal{P}$, and the symbol $< 0 >$ denotes the sum over the lattice vectors that are nearest to the origin; i.e., nearest neighbor. We assume that if the site $\mathbf{v}$ is in the set $< 0 >$ then so is $-\mathbf{v}$, which, writing (9) as

$$i\frac{d}{d\tau}\vec{a} = \mathcal{L}_{sim}\vec{a} + \sigma\tilde{\mathcal{N}}(\vec{a}),$$

makes the bounded linear operator $\mathcal{L}_{sim}$ self adjoint. The coefficient $\lambda_{\mathbf{v}}$ is defined by

$$\lambda_{\mathbf{v}} = \left\langle \frac{\tilde{\delta}V_{orb}}{h^2}\phi, \phi_{\mathbf{v}} \right\rangle,$$

where $< \cdot, \cdot >$ denotes the $L^2(\mathbb{R}^2)$ inner product. Equation (9) is usually referred to as the discrete NLS equation. Note, given our choice of ϵ, the dynamical system for the coefficients $a_{\mathbf{p}}$ is maximally balanced.

It can be shown that for any $p \geq 0$, if one has an initial vector $\mathbf{a}_0$, in $l^2_s(\mathcal{P})$, $s \geq 0$, then there is a corresponding solution $\mathbf{a}(\tau)$ in $C^1(\mathbb{R}, l^2_s(\mathcal{P}))$ (see e.g. Lemma 6 in[17] which presents a means of establishing this result using energy

methods). Since we want the solutions to the discrete system to also be in $l^1(\mathcal{P})$, one needs to take $s > 1$. This result also holds for the discrete system (18).

4. Solving for the remainder $R(\mathbf{r}, z)$

In this section, we assume that the sequence $a_{\mathbf{v}}$ is in l^1. Using the ansatz for ϕ_w in (8), we rewrite (8) as a nonlinear nonautonomous problem in solving for the remainder R. Thus (8) becomes

$$\begin{aligned} &i\epsilon^{\alpha} R_z - \epsilon^{\alpha}(L_h - \mu_0(\mathbf{k}))R + G(\phi_w) \\ &+\frac{\sigma\epsilon}{g}\left(|\phi_w + \epsilon^{\alpha}R|^2(\phi_w + \epsilon^{\alpha}R) - g\sum_{\mathbf{p}}|a_{\mathbf{p}}|^2 a_{\mathbf{p}}\phi_{\mathbf{p}}\right) = 0, \end{aligned} \tag{10}$$

with

$$G(\phi_w) = \sum_{\mathbf{p}}\left(a_{\mathbf{p}}\frac{\tilde{\delta}V_{orb,\mathbf{p}}}{h^2} - \sum_{<0>} a_{\mathbf{p}+\mathbf{v}}\lambda_{\mathbf{v}}\right)\phi_{\mathbf{p}},$$

where $\tilde{\delta}V_{orb,\mathbf{p}}(\mathbf{r}) = \tilde{\delta}V_{orb}(\mathbf{r} - \mathbf{p})$, and $\chi_{\mathbf{p}}(\mathbf{r}) = \chi(\mathbf{r} - \mathbf{p})$. Controlling $G(\phi_w)$ follows from Lemma 2, and one then has that

$$||G(\phi_w)||_{H_2(\mathbb{R}^2)} = \mathcal{O}(\epsilon). \tag{11}$$

If one defines $\mathcal{N}(\phi_w, R)$ by

$$\mathcal{N}(\phi_w, R) = \frac{\sigma}{g}\left(|\phi_w + \epsilon^{\alpha}R|^2(\phi_w + \epsilon^{\alpha}R) - g\sum_{\mathbf{p}}|a_{\mathbf{p}}|^2 a_{\mathbf{p}}\phi_{\mathbf{p}}\right),$$

then we rewrite (10), noting that $R(\mathbf{r}, 0) = 0$, in the Duhamel form

$$R(\mathbf{r}, z) = -i\int_0^z T(z - t')(\epsilon^{-\alpha}G(\phi_w) + \epsilon^{1-\alpha}\mathcal{N}(\phi_w, R))dt', \tag{12}$$

where $T(t)$ is the $L^2(\mathbb{R}^2)$-unitary group operator generated by the self-adjoint operator $-i(L_h - \mu_0(\mathbf{k}))$. Then we define the nonlinear operator

$$\mathcal{B}(W) = -i\int_0^z T(z - t')(\epsilon^{-\alpha}G(\phi_w) + \epsilon^{1-\alpha}(\mathcal{N}(\phi_w, W))dt',$$

and further, we define the metric space

$$B_{\Gamma}(\tilde{Z}) = \left\{W \in C([0, \tilde{Z}); H_2(\mathbb{R}^2)) : \sup_{z\in[0,\tilde{Z})} ||W(\cdot, z)||_{H_2(\mathbb{R}^2)} \leq \Gamma\right\},$$

and the norm

$$|||W||| = \sup_{z\in[0,\tilde{Z})} ||W(\cdot,z)||_{H_2(\mathbb{R}^2)}.$$

There exist constants C_1, C_2, and C_3 such that

$$|||\mathcal{B}(W)||| \le \epsilon^{1-\alpha}\tilde{Z}C_1 + \epsilon\tilde{Z}C_2|||W||| + \epsilon^{1+\alpha}\tilde{Z}C_3|||W|||^2 + \epsilon^{1+2\alpha}\tilde{Z}|||W|||^3$$

Thus, if one wants

$$\sup_{z\in[0,\tilde{Z})} ||\mathcal{B}(W)(\cdot,z)||_{H_2(\mathbb{R}^2)} \le \Gamma,$$

then for any time $\tilde{Z}$, one need only choose ϵ sufficiently small to ensure the desired condition.

One also has for $Y, W \in B_\Gamma(\tilde{Z})$ that

$$|||\mathcal{B}(W) - \mathcal{B}(Y)||| \le$$

$$\left(3\epsilon||\phi_w||^2 + 8\epsilon^{1+\alpha}||\phi_w||\Gamma + 3\epsilon^{1+2\alpha}\Gamma^2\right)|||W - Y|||.$$

Thus, for given Γ and h sufficiently small, $\mathcal{B}(\cdot)$ is a contraction. So by the Banach Fixed-Point Theorem, we have a unique solution R to (12) with

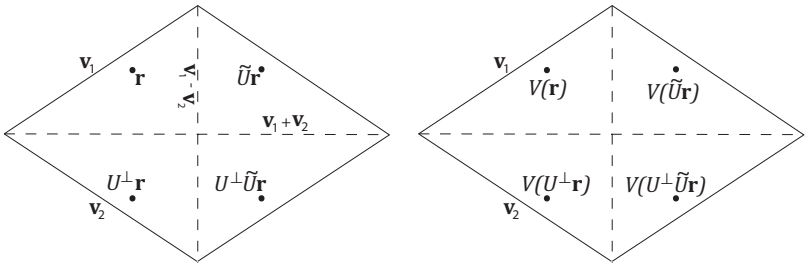
$$|||R||| \le \Gamma$$

for z-scales on the order of $\mathcal{O}(\epsilon^{\alpha-1})$. Thus the Theorem for simple lattices in the Introduction of the paper is proved. In the next section this Theorem is extended to non-simple HC lattices.

5. Non-simple honeycomb lattices

In this section, we outline the rigorous justification of the tight-binding approximation in non-simple HC lattices; the necessary arguments follow closely those in the preceding text. We highlight the differences and complications that arise relative to the simple lattice case in the context of the work in [7] and provide a brief argument showing how Theorem 1 extends to the non-simple HC case.

For non-simple HC lattices, we assume that the vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ are equal in magnitude so that $\mathbf{v}_1 + \mathbf{v}_2$ is orthogonal to $\mathbf{v}_1 - \mathbf{v}_2$. We further assume that $|\mathbf{v}_1 + \mathbf{v}_2| \ge |\mathbf{v}_1 - \mathbf{v}_2|$, and that one corner of Ω is set at the origin so that the center of Ω is given by $(\mathbf{v}_1 + \mathbf{v}_2)/2$. The potential V is still periodic, but now we assume it has two wells within the fundamental cell Ω, one at $\mathbf{r}_1$, the other at $\mathbf{r}_2$. We define the seperation vector $\mathbf{d} = \mathbf{r}_2 - \mathbf{r}_1$, and for clarity we choose $\mathbf{r}_1$ and $\mathbf{r}_2$ such that $\mathbf{r}_1 + \mathbf{r}_2 = \mathbf{v}_1 + \mathbf{v}_2$. This choice forces us to add the



(a) Reflection Maps (b) Potential Symmetries

Figure 4. Symmetry relationships in Ω; points in figures denote locations and values of potentials, respectively.

constraint that $|\mathbf{d}| < |\mathbf{v}_1 + \mathbf{v}_2|/2$, since otherwise we could redefine $\mathbf{v}_1$ and $\mathbf{v}_2$ to get a new lattice with a smaller distance between the wells.

One way to build such a potential is to choose a smooth function of compact support, say $V_b(\mathbf{r})$, where the support of V_b is chosen to be on a triangle similar to the lower half of Ω. We likewise assume that $V_b(\mathbf{r}_1) = 0$ and otherwise $V_b(\mathbf{r}) > 0$ except at the boundary of the support. Define the Householder projection U across $\mathbf{v}_1 - \mathbf{v}_2$ as

$$U\mathbf{r} = \mathbf{r} - 2 \operatorname{proj}_{\mathbf{v}_1+\mathbf{v}_2}\mathbf{r}.$$

We also define the complementary projection $U^\perp$ that represents reflection across $\mathbf{v}_1 + \mathbf{v}_2$ by

$$U^\perp\mathbf{r} = \mathbf{r} - 2 \operatorname{proj}_{\mathbf{v}_1-\mathbf{v}_2}\mathbf{r}.$$

See Figure 4a for clarification. We further assume that $V_b(U^\perp\mathbf{r}) = V_b(\mathbf{r})$. We then define $\tilde{V}_b(\mathbf{r})$ to be the mirror image of $V(\mathbf{r})$ across the line $\mathbf{v}_1 - \mathbf{v}_2$, i.e., let $\tilde{V}_b(\mathbf{r}) = V_b(\tilde{U}\mathbf{r})$ with $\tilde{U}\mathbf{r} = \mathbf{v}_1 + \mathbf{v}_2 + U\mathbf{r}$. We define $V(\mathbf{r})$ to be

$$V(\mathbf{r}) = \sum_{\mathbf{v}\in\mathcal{P}} V_b(\mathbf{r} - \mathbf{v}) + \tilde{V}_b(\mathbf{r} - \mathbf{v}). \tag{13}$$

We must be sure to choose the support of $V_b(\mathbf{r})$ so that no extra wells are introduced while also having only one well in each triangular support. We assume throughout the rest of the section that $V(\mathbf{r})$ is of the form (13). Thus the potential around every well is identical, but the positions of the wells are not strictly related to each other in a periodic way. Likewise, since $\tilde{U}^2 = I$, we have that $V(\tilde{U}\mathbf{r}) = V(\mathbf{r})$, and since $U^\perp\tilde{U} = \tilde{U}U^\perp$, $V(U^\perp\mathbf{r}) = V(\mathbf{r})$. Thus at each of the four labeled points in Figure 4b the potential $V(\mathbf{r})$ has the same value.

We then choose some value η_0 sufficiently small so that in the ball around $\mathbf{r}_1$, say $B_A(\mathbf{r}_1, \eta_0)$, defined by the Agmon metric, we have only the well $\mathbf{r}_1$ and not $\mathbf{r}_2$. Define $B_A(\mathbf{r}_2, \eta_0)$ in a similar fashion. Further, choose η_0 such that the

balls are disjoint. Then, choose a point $\mathbf{r}$ such that $d_A(\mathbf{r}, \mathbf{r}_1) < \eta_0$. We choose a path $\gamma(t)$ such that $\gamma(0) = \mathbf{r}_2 = \tilde{U}\mathbf{r}_1$ and $\gamma(1) = \tilde{U}\mathbf{r}$. Then we have that

$$\int_0^1 \sqrt{V(\gamma(t))}|\dot{\gamma}|dt = \int_0^1 \sqrt{V(\tilde{U}\tilde{\gamma}(t))}\left|\frac{d(\tilde{U}\tilde{\gamma})}{dt}\right| dt = \int_0^1 \sqrt{V(\tilde{\gamma}(t))}|\dot{\tilde{\gamma}}|dt,$$

where $\tilde{\gamma}(t)$ is a path such that $\tilde{\gamma}(0) = \mathbf{r}_1$ and $\tilde{\gamma}(1) = \mathbf{r}$, and we have used that

$$\left|\frac{d(\tilde{U}\tilde{\gamma})}{dt}\right| = \left|U\frac{d\tilde{\gamma}}{dt}\right| = \left|\frac{d\tilde{\gamma}}{dt}\right|,$$

since U is unitary. Taking the infimum over all paths we see that $d_A(\tilde{U}\mathbf{r}, \mathbf{r}_2) = d_A(\mathbf{r}, \mathbf{r}_1) < \eta_0$, so that each ball $B_A(\mathbf{r}_j, \eta_0)$ is the image of the other under the mapping $\tilde{U}$. We also note that $U^{\perp}\mathbf{r}_j = \mathbf{r}_j$, so that using an argument essentially identical to that just used, we have $U^{\perp}B_A(\mathbf{r}_j, \eta_0) = B_A(\mathbf{r}_j, \eta_0)$.

We define the potential

$$V_1 = V + (1 - \chi),$$

where χ is a smooth function of compact support within $B_A(\mathbf{r}_1, \eta_0)$, $0 \leq \chi \leq 1$, and $\chi|_{B_A(\mathbf{r}_1, \frac{\eta_0}{2})} = 1$. Following [7], we define the second potential

$$V_2(\mathbf{r}) = V_1(\tilde{U}\mathbf{r}) = V(\mathbf{r}) + 1 - \chi(\tilde{U}\mathbf{r}),$$

where we have used the fact that $V(\tilde{U}\mathbf{r}) = V(\mathbf{r})$. If $\chi(\mathbf{r})$ has support on $B_A(\mathbf{r}_1, \eta_0)$, then using previous arguments, we see that $\chi(\tilde{U}\mathbf{r})$ has support on $B_A(\mathbf{r}_2, \eta_0)$ since $B_A(\mathbf{r}_1, \eta_0) = \tilde{U}B_A(\mathbf{r}_2, \eta_0)$.

We define $\tilde{\delta}V_1 = V_1 - V$ and $\tilde{\delta}V_2 = V_2 - V$. By construction then, both V_1 and V_2 are one-well potentials, and we define the two orbitals, ϕ_1 and ϕ_2, via the eigenvalue problems

$$-\Delta\phi_j + \frac{1}{h^2}V_j\phi_j = \tilde{E}_0\phi_j \tag{14}$$

for $j = 1, 2$. Note the eigenvalues are identical since $V_2(\mathbf{r}) = V_1(\tilde{U}\mathbf{r})$, and the Laplacian is invariant under shifts and unitary transformations in $\mathbf{r}$. This also shows that $\phi_2(\mathbf{r}) = \phi_1(\tilde{U}\mathbf{r})$, or if ϕ_1 is localized around $\mathbf{r}_1$ then ϕ_2 is localized around $\mathbf{r}_2$. Further, since $V_j(U^{\perp}\mathbf{r}) = V_j(\mathbf{r})$ by construction, and since $U^{\perp}$ is unitary, we also have $\phi_j(U^{\perp}\mathbf{r}) = \phi_j(\mathbf{r})$, which means the orbital functions are symmetric around each well.

We use ϕ_1 and ϕ_2 to build a tight-binding approximation to solve (1). To this end, we first prove the following theorem.

THEOREM 5. *Let* $\mathbf{r}_1, \mathbf{r}_2$ *be two neighboring potential minima. Then the dispersion relations (eigenvalues) of* $L_{h,\mathbf{k}}$ *satisfy*

$$\mu_l(\mathbf{k}) = \tilde{E}_0 + \mathcal{O}\left(\frac{e^{-(d_A(\mathbf{r}_1,\mathbf{r}_2)-\delta)/h}}{h^2}\right)$$

with $d_A(\mathbf{r}_1, \mathbf{r}_2) - \delta > 0$, *for* $l = 0$ *or* 1 *and uniformly for* $\mathbf{k} \in \Omega'$ *with* $\delta > 0$ *being a parameter determined by the lattice.*

Proof: To prove this theorem requires more machinery than in the case of simple lattices. Our approach is to first approximate the eigenvalues $\mu_l(\mathbf{k})$ by the eigenvalues of a restriction of the operator L_h to a compact domain. Then we approximate the eigenvalues of the compactly defined operator by those of the operator defining the orbitals which proves the theorem.

Following [9], we denote the set of wells as $\mathcal{W} = \{\mathbf{r}_1, \mathbf{r}_2\}$, and we define the function $d_A(\mathbf{r}, \mathcal{W})$ as

$$d_A(\mathbf{r}, \mathcal{W}) = \inf_{\mathbf{r}' \in \mathcal{W}} d_A(\mathbf{r}, \mathbf{r}').$$

We define the constant S_0 such that

$$S_0 = \min\left\{\inf_{\mathbf{v}\neq 0} d_A(\mathbf{r}_1, \mathcal{W} + \mathbf{v}), \inf_{\mathbf{v}\neq 0} d_A(\mathbf{r}_2, \mathcal{W} + \mathbf{v})\right\},$$

where $\mathbf{v}$ is a lattice vector (i.e., S_0 is the distance to the next closest well to either $\mathbf{r}_1$ or $\mathbf{r}_2$ as measured in the Agmon metric). We define the domain M_0 as a bounded domain with smooth boundary such that the closure of every ball $B_A(\mathcal{W}, S)$, $S < S_0$, is in the interior of M_0. Note the ball $B_A(\mathcal{W}, S)$ is defined as

$$B_A(\mathcal{W}, S) = \left\{\mathbf{r} \in \mathbb{R}^2 : \inf_{\mathbf{r}' \in \mathcal{W}} d_A(\mathbf{r}, \mathbf{r}') < S\right\},$$

and $M_0 \cap (\mathcal{W} + \mathbf{v}) = \emptyset$ for $\mathbf{v} \neq 0$. Hence M_0 contains the two wells $\mathbf{r}_1$ and $\mathbf{r}_2$. Further, given that $V(\tilde{U}\mathbf{r}) = V(\mathbf{r})$, we have that $\tilde{U}M_0 = M_0$. This can be seen by repeating the argument used above to establish the equivalence of the balls $B_A(\mathbf{r}_j, \eta_0)$.

We define the operator L_{h,M_0} as the restriction of L_h to the domain $H_2(M_0) \cap H_{1,0}(M_0)$. Note, the Sobolev spaces $H_{1,0}(M_0)$ and $H_2(M_0)$ are functions with one and two weak derivatives that are in $L^2(M_0)$. Likewise the trace of the functions in $H_{1,0}(M_0)$ vanish along the boundary of M_0. See [23] for more details on these Sobolev spaces and the definition of the trace of a function. Now suppose there exists some interval $I(h)$, such that the operator L_{h,M_0} has m eigenvalues, $\tilde{\lambda}_l(h)$, $0 \leq l \leq m-1$, in $I(h)$ with the remainder of its spectrum some nonexponentially small distance away from $I(h)$. We can then use the following theorem from [9].

There exists some value $S_1 < S_0$ *such that if there are* m *eigenvalues of* L_{h,M_0} *in an interval* $I(h)$, *then there are* m *eigenvalues of* $L_{h,\mathbf{k}}$ *in* $I(h)$, *and*

we have the uniform in $\mathbf{k}$ *asymptotic expansion*

$$\mu_l(\mathbf{k}) = \tilde{\lambda}_l + \mathcal{O}\left(\frac{e^{-S_1/h}}{h^2}\right), \tag{15}$$

for $0 \leq l \leq m-1$.

As indicated above, by construction the domain M_0 contains exactly two wells. Choosing $\eta_0 < S_0$, we define the punctured domains $W_1 = M_0 \backslash B_A(\mathbf{r}_2, \eta_0)$ and $W_2 = M_0 \backslash B_A(\mathbf{r}_1, \eta_0)$. Given the symmetry of V with respect to $\tilde{U}$, we have that

$$V|_{W_2}(\mathbf{r}) = V|_{W_1}(\tilde{U}\mathbf{r}),$$

and therefore the eigenvalues of the operators L_{h,W_j} are the same for both $j = 1, 2$ since $\tilde{U}$ is composed of a constant shift and a unitary matrix. Denoting the ground state eigenvalue of L_{h,W_j}, corresponding to an eigenvector having zero Dirichlet data, as $\tilde{\lambda}_w$, each spectral problem for L_{h,W_j} is a single-well problem, and therefore from [21] we have that $\tilde{\lambda}_w$ is $\mathcal{O}(1/h)$ and can be isolated from the remainder of the spectrum of L_{h,W_j} within some interval $I(h)$. Using the argument from Lemma 6.11 in [21], we can show the first two eigenvalues $\tilde{\lambda}_0$ and $\tilde{\lambda}_1$ of L_{h,M_0} are exponentially close with

$$\tilde{\lambda}_0 = \tilde{\lambda}_w - w + \cdots$$
$$\tilde{\lambda}_1 = \tilde{\lambda}_w + w + \cdots,$$

where

$$w = \mathcal{O}\left(\frac{e^{-(d_A(\mathbf{r}_1,\mathbf{r}_2)-\delta)/h}}{h^2}\right),$$

with $\delta > 0$ and C a constant. Thus, if we choose δ such that $0 < d_A(\mathbf{r}_1, \mathbf{r}_2) - \delta \leq S_1$, using (15), one sees that there is an exponential splitting between the two lowest bands of the periodic problem, with the order of the splitting being controlled by the interwell spacing. Note, if $d_A(\mathbf{r}_1, \mathbf{r}_2) < S_1$, δ remains a free parameter.

In order to connect back to the orbitals, we compute that

$$\left(-\Delta + \frac{1}{h^2}\, V|_{W_j}\right)\chi_j\phi_j = \tilde{E}_0\chi_j\phi_j + \frac{\tilde{\delta}V_j}{h^2}\chi_j\phi_j - [\Delta, \chi_j]\phi_j,\ j = 1, 2. \tag{16}$$

Note, we have, since $B_A(\mathbf{r}_j, \eta_0) \subset W_j$, that

$$V|_{W_j}(\chi_j\phi_j) = (V_j + \tilde{\delta}V_j)(\chi_j\phi_j),\ j = 1, 2.$$

Using Theorem 3, it follows for $j = 1, 2$ that

$$||\tilde{\delta}V_j\chi_j\phi_j||_{L^2(\mathbb{R}^2)} = \mathcal{O}(e^{(-(1-\bar{\delta})b_{0,j}+\bar{\delta})/h}),$$
$$||[\Delta, \chi_j]\phi_j||_{L^2(\mathbb{R}^2)} = \mathcal{O}(e^{(-(1-\bar{\delta})b_{0,j}+\bar{\delta})/h}),$$

where $\bar{\delta} > 0$ and

$$b_{0,j} = \inf_{\mathbf{r} \in \tilde{B}_j} d_A(\mathbf{r}, \mathbf{r}_j)$$

with

$$\tilde{B}_j = B_A(\mathbf{r}_j, \eta_0) \backslash B_A(\mathbf{r}_j, \eta_0/2),$$

so we can take $b_{0,j} = \frac{\eta_0}{2}$, $j = 1, 2$. We assume $b_{0,1} = b_{0,2}$ and that $\bar{\delta}$, η_0, and δ are chosen such that

$$(1 - \bar{\delta})\frac{\eta_0}{2} - \bar{\delta} = d_A(\mathbf{r}_1, \mathbf{r}_2) - \delta.$$

Note, there is a limitation to how large η_0 can be since we require that $B_A(\mathbf{r}_1, \eta_0)$ and $B_A(\mathbf{r}_2, \eta_0)$ be disjoint. Then using Lemma 3.2 from [9], we have, for $l = 0$ or 1 that

$$\tilde{\lambda}_l = \tilde{E}_0 + \mathcal{O}\left(\frac{e^{-(d_A(\mathbf{r}_1, \mathbf{r}_2) - \delta)/h}}{h^2}\right)$$

and so

$$\mu_l(\mathbf{k}) = \tilde{E}_0 + \mathcal{O}\left(\frac{e^{-(d_A(\mathbf{r}_1, \mathbf{r}_2) - \delta)/h}}{h^2}\right)$$

for $l = 0$ or 1 and uniformly for $\mathbf{k} \in \Omega'$. ■

Thus we have shown that there is an exponentially small splitting in the first two bands of the periodic problem and further that the leading order behavior of both can be described by the eigenvalues of the orbital problem. Note, one could in principle derive a rigorous theory showing the exponential splitting using orbitals alone. However, this is beyond the scope of the present paper.

Going further, suppose that there is a value $\mathbf{k}$ such that $\mu_0(\mathbf{k}) = \mu_1(\mathbf{k})$, i.e., the two bands touch. Such a value of $\mathbf{k}$ is called a Dirac point [7]. We now describe a number of quantities necessary to build a tight-binding approximation at a Dirac point. Define the quantity

$$c_0 = \left\langle \frac{\tilde{\delta} V_1}{h^2}\phi_1, \phi_1 \right\rangle = \left\langle \frac{\tilde{\delta} V_2}{h^2}\phi_2, \phi_2 \right\rangle,$$

where the equality comes from ϕ_2 and $\tilde{\delta} V_2$ being translations and unitary transformations of ϕ_1 and $\tilde{\delta} V_1$. Further, in the case of a non-simple HC lattice, each well has three nearest neighbors (see Figure 5). Thus we have, when $\mathbf{p} \neq 0$,

$$< \phi_{1,\mathbf{q}}, \phi_{1,\mathbf{p}} > = < \phi_{2,\mathbf{q}}, \phi_{2,\mathbf{p}} > \ll < \phi_{1,\mathbf{p}}, \phi_{2,\mathbf{p}} > \ll 1,$$

where $\phi_{j,\mathbf{p}}(\mathbf{r}) = \phi_j(\mathbf{r} - \mathbf{p})$ for $j = 1, 2$, and $\mathbf{q} \neq \mathbf{p}$. We also have that

$$< \phi_1, \phi_{2,-\mathbf{v}_2} >, < \phi_1, \phi_{2,-\mathbf{v}_1} > \gg < \phi_1, \phi_{1,\mathbf{p}} >,$$

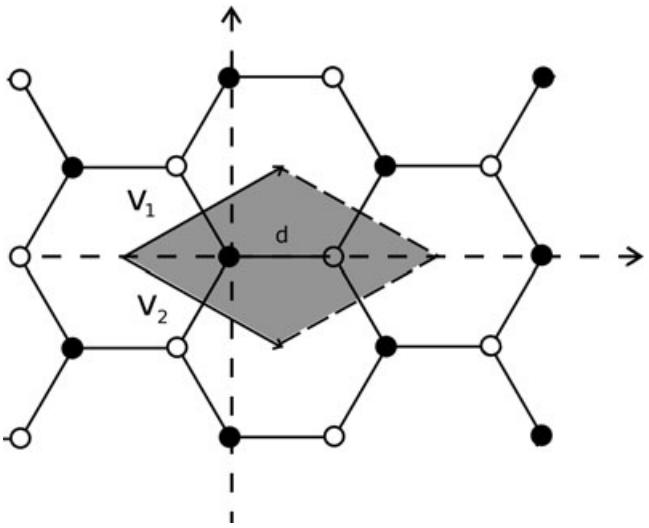


Figure 5. Nearest neighbor interactions.

Note, a similar argument can be made relative to the well $\mathbf{r}_2$. These results state that nearest neighbor interactions are asymptotically dominant (again see Figure 5 for clarification). While we do not prove these relationships, given the asymptotic behavior of the orbitals as shown in Section 6, it is clear that the results will hold. Further, we only use the fact that all of these terms are small in the following theorem. See Figure 5 for reference.

To get control over the term $< \phi_{1,\mathbf{p}}, \phi_{2,\mathbf{p}} >$, by decomposing integrals over different balls around the wells we have

$$\int_{\mathbb{R}^2} \phi_1 \phi_2 d\mathbf{r} = \int_{B_{A,1}} \phi_1 \phi_2 d\mathbf{r} + \int_{B_{A,2}} \phi_1 \phi_2 d\mathbf{r} + \int_{\mathbb{R}^2 \setminus \bar{B}} \phi_1 \phi_2 d\mathbf{r}, \tag{17}$$

where $B_{A,j} = B_A(\mathbf{r}_j, \eta_0)$ and $\bar{B} = B_{A,1} \cup B_{A,2}$. Note, we now have for example

$$\left| \int_{B_{A,1}} \phi_1 \phi_2 d\mathbf{r} \right| = \left| \int_{B_{A,1}} \phi_1(\mathbf{r}) \phi_1(\tilde{U}\mathbf{r}) d\mathbf{r} \right| \leq C_{\delta_{12}} e^{-((1-\delta_{12})b_{12} - \delta_{12})/h},$$

where $0 < \delta_{12} < 1$, and using Theorem 3, we define b_{12} to be

$$b_{12} = \inf_{\mathbf{r} \in B_{A,1}} d_A(\tilde{U}\mathbf{r}, \mathbf{r}_1).$$

Repeating the arguments from Lemma 2 shows that $< \phi_{1,\mathbf{p}}, \phi_{2,\mathbf{p}} >= \mathcal{O}(e^{-\tilde{b}/h})$ where

$$\tilde{b} = \min \left\{ \inf_{\mathbf{r} \in B_{A,1}} d_A(\mathbf{r}, \mathbf{r}_2), \inf_{\mathbf{r} \in B_{A,2}} d_A(\mathbf{r}, \mathbf{r}_1), \inf_{\mathbf{r} \in \mathbb{R}^2 \setminus \bar{B}} d(\mathbf{r}, \mathcal{W}) \right\}.$$

So, as in the simple lattice case, $\tilde{b}(\eta_0)$ tends to zero as η_0 goes to zero or infinity. Comparing this fact to the requirement from above that one must have $(1-\bar{\delta})\frac{\eta_0}{2} - \bar{\delta} = d_A(\mathbf{r}_1, \mathbf{r}_2) - \delta$, then we first note that as one takes $\bar{\delta}$ to zero, then the line $(1-\bar{\delta})\frac{\eta_0}{2} - \bar{\delta}$ must intersect $\tilde{b}(\eta_0)$ at smaller and smaller values of η_0. As with simple lattices, this conveniently chooses η_0. Choosing δ sufficiently large then ensures that all three terms balance and we can still satisfy the condition $0 < d_A(\mathbf{r}_1, \mathbf{r}_2) - \delta \leq S_1$. The smallness of the other terms can be established in a similar fashion.

With these definitions and results in hand then, a tight-binding approximation ϕ_w is constructed in [7] where ϕ_w is given by

$$\phi_w(\mathbf{r}, z) = \sum_{\mathbf{p}} a_{\mathbf{p}}(\epsilon z)\phi_1(\mathbf{r} - \mathbf{p}) + b_{\mathbf{p}}(\epsilon z)\phi_2(\mathbf{r} - \mathbf{p}).$$

Then we approximate a solution to the NLS equation via

$$u_{hc}(\mathbf{r}, z) = \sqrt{\frac{\epsilon}{g}}\phi_w(\mathbf{r}, z)e^{-i(\tilde{E}_0 - c_0)z},$$

with

$$\epsilon = \mathcal{O}\left(\frac{e^{-(d_A(\mathbf{r}_1,\mathbf{r}_2)-\delta)/h}}{h^4}\right).$$

We introduce the constants (see also [7])

$$c_1 = < \phi_1, \phi_2 >,$$
$$c_2 = < \tilde{\delta} V_1 \phi_1, \phi_2 > \ = < \tilde{\delta} V_2 \phi_2, \phi_1 > .$$

and

$$\rho_1 = \frac{< \phi_1, \phi_{2,-\mathbf{v}_j} >}{c_1} = \frac{< \phi_2, \phi_{1,\mathbf{v}_j} >}{c_1},$$
$$\rho_2 = \frac{< \tilde{\delta} V_2 \phi_2, \phi_{1,\mathbf{v}_j} >}{c_2} = \frac{< \tilde{\delta} V_1 \phi_1, \phi_{2,-\mathbf{v}_j} >}{c_2},$$

where $j = 1, 2$, and we have taken ρ_1 and ρ_2 to be independent of the choice of $\mathbf{v}_1$ or $\mathbf{v}_2$.

We can show the above equalities in the following way. Note that $U(\mathbf{v}_j) = -\mathbf{v}_i$, where U is the Householder projection and $\phi_2(\mathbf{r}) = \phi_1(\tilde{U}\mathbf{r})$. Then we have that

$$< \phi_1, \phi_{2,-\mathbf{v}_1} > = \int_{\mathbb{R}^2} \phi_1(\mathbf{r})\phi_1(\tilde{U}(\mathbf{r} + \mathbf{v}_1))d\mathbf{r},$$

$$= \int_{\mathbb{R}^2} \phi_1(\mathbf{r})\phi_1(\tilde{U}\mathbf{r} - \mathbf{v}_2)d\mathbf{r},$$

$$= \int_{\mathbb{R}^2} \phi_1(\tilde{U}\mathbf{r})\phi_1(\mathbf{r} - \mathbf{v}_2)d\mathbf{r}.$$

In the last step, the coordinate change $\mathbf{r} \to \tilde{U}\mathbf{r} = U\mathbf{r} + \mathbf{v}_1 + \mathbf{v}_2$ was used, where we note again that $\tilde{U}^2 = I$, and since U is unitary, the Jacobian of the coordinate change is one. Therefore, using previous definitions, we then have that

$$< \phi_1, \phi_{2,-\mathbf{v}_1} >=< \phi_{1,\mathbf{v}_2}, \phi_2 >=< \phi_1, \phi_{2,-\mathbf{v}_2} > .$$

Thus ρ_1 is well defined and independent of the choice of $\mathbf{v}_j$. Using a similar argument shows c_2 is well defined. We then note that

$$\begin{aligned}
< \tilde{\delta} V_2 \phi_2, \phi_{1,\mathbf{v}_j} >&= \int_{\mathbb{R}^2} \tilde{\delta} V_1(\tilde{U}\mathbf{r}) \phi_1(\tilde{U}\mathbf{r}) \phi_1(\mathbf{r} - \mathbf{v}_j) d\mathbf{r}, \\
&= \int_{\mathbb{R}^2} \tilde{\delta} V_1(\mathbf{r}) \phi_1(\mathbf{r}) \phi_1(\tilde{U}\mathbf{r} - \mathbf{v}_j) d\mathbf{r}, \\
&= \int_{\mathbb{R}^2} \tilde{\delta} V_1(\mathbf{r}) \phi_1(\mathbf{r}) \phi_1(\tilde{U}(\mathbf{r} + \mathbf{v}_i)) d\mathbf{r}, \\
&= \int_{\mathbb{R}^2} \tilde{\delta} V_1(\mathbf{r}) \phi_1(\mathbf{r}) \phi_2(\mathbf{r} + \mathbf{v}_i) d\mathbf{r}, \\
&=< \tilde{\delta} V_1 \phi_1, \phi_{2,-\mathbf{v}_i} > .
\end{aligned}$$

From this equality, noting that $U^{\perp}\mathbf{v}_j = \mathbf{v}_i$ and $\phi_j(U^{\perp}\mathbf{r}) = \phi_j(\mathbf{r})$, we also get

$$\begin{aligned}
< \tilde{\delta} V_2 \phi_2, \phi_{1,\mathbf{v}_j} >&= \int_{\mathbb{R}^2} \tilde{\delta} V_1(\mathbf{r}) \phi_1(\mathbf{r}) \phi_2(\mathbf{r} + \mathbf{v}_i) d\mathbf{r}, \\
&= \int_{\mathbb{R}^2} \tilde{\delta} V_1(U^{\perp}\mathbf{r}) \phi_1(U^{\perp}\mathbf{r}) \phi_2(U^{\perp}\mathbf{r} + \mathbf{v}_j) d\mathbf{r}, \\
&= \int_{\mathbb{R}^2} \tilde{\delta} V_1(\mathbf{r}) \phi_1(\mathbf{r}) \phi_2(U^{\perp}(\mathbf{r} + \mathbf{v}_i)) d\mathbf{r}, \\
&=< \tilde{\delta} V_1 \phi_1, \phi_{2,-\mathbf{v}_j} > .
\end{aligned}$$

We have therefore shown that all of the equalities are a consequence of the symmtries of the potential and are well-defined and independent of the choice of $\mathbf{v}_j$.

Using the nearest neighbor arguments presented above, inserting the expression for ϕ_w into the lattice NLS equation, and taking inner products with respect to both $\phi_{1,\mathbf{p}}$ and $\phi_{2,\mathbf{p}}$, yields a dynamical system for the coefficients $a_{\mathbf{p}}$

and $b_{\mathbf{p}}$ in the form

$$\begin{aligned} i\epsilon\dot{a}_{\mathbf{p}} + (c_0c_1\mathcal{L}_1^- - c_2\mathcal{L}_2^-)b_{\mathbf{p}} + \sigma\epsilon|a_{\mathbf{p}}|^2a_{\mathbf{p}} = 0, \\ i\epsilon\dot{b}_{\mathbf{p}} + (c_0c_1\mathcal{L}_1^+ - c_2\mathcal{L}_2^+)a_{\mathbf{p}} + \sigma\epsilon|b_{\mathbf{p}}|^2b_{\mathbf{p}} = 0, \end{aligned} \tag{18}$$

where, for $n = 1$ or 2,

$$\begin{aligned} \mathcal{L}_n^- b_{\mathbf{p}} &= b_{\mathbf{p}} + \rho_n b_{\mathbf{p}-\mathbf{v}_1} + \rho_n b_{\mathbf{p}-\mathbf{v}_2}, \\ \mathcal{L}_n^+ a_{\mathbf{p}} &= a_{\mathbf{p}} + \rho_n a_{\mathbf{p}+\mathbf{v}_1} + \rho_n a_{\mathbf{p}+\mathbf{v}_2}. \end{aligned}$$

This system of equations, termed the discrete Dirac system, is markedly different from the simple lattice case, and in a continuum limit leads to another Dirac system. See [7] for more details. In terms of establishing a result akin to Theorem 1 in the simple lattice case, one need only note that the coefficients in the terms $\mathcal{L}_n^-$ and $\mathcal{L}_n^+$ are $\mathcal{O}(\epsilon)$, and therefore the analogous term $G(\phi_w)$ (see (10)) is small. Thus for non-simple HC lattices we have established

THEOREM 6. *Let $\tilde{b} > 0$ be some constant and define*

$$\epsilon = \frac{e^{-\tilde{b}/h}}{h^4},$$

and choose coefficients $a_{\mathbf{v},0}$ and $b_{\mathbf{v},0}$ such that $\{a_{\mathbf{v},0}\}_{\mathbf{v}\in\mathcal{P}}$ and $\{b_{\mathbf{v},0}\}_{\mathbf{v}\in\mathcal{P}}$ are in l_s^2, $s > 1$. Then, for a non-simple HC lattice, for h sufficiently small, there exists a solution to (1), $u(\mathbf{r}, z)$, such that

$$||u(\mathbf{r}, z) - u_{hc}(\mathbf{r}, z)||_{H_2(\mathbb{R}^2)} = \mathcal{O}(\epsilon^{\frac{1}{2}+\alpha})$$

for values z such that $z = \mathcal{O}(\epsilon^{-1+\alpha})$, where $0 < \alpha < 1$.

Note, we have expanded u as

$$u(\mathbf{r}, z) = \sqrt{\frac{\epsilon}{g}}\left(u_{hc}(\mathbf{r}, z) + \epsilon^{\alpha}R(\mathbf{r}, z)e^{-i(\tilde{E}_0 - c_0)z}\right),$$

where $g = ||\phi||_{L^4(\mathbb{R}^2)}^4$, and $0 < \alpha < 1$.

6. WKB approximations of orbitals

On a final note, it is desirable to find constructive approximations to the orbital functions ϕ_j such that replacing the orbital functions with these approximations yields an equivalent statement to Theorem 6. A method for doing that is the following. Using the balls $B_A(\mathbf{r}_1, \eta_0)$ and $B_A(\mathbf{r}_2, \eta_0)$ described above, we study the eigenvalue problems $L_{h,B_A(\mathbf{r}_j,\eta_0)}$. We assume there is a symmetry such that these eigenvalue problems are the same modulo shifting by $\mathbf{d}$. We define the eigenvalue and eigenfunction associated with this problem as $\tilde{\lambda}_b$ and $\tilde{\varphi}_b$,

respectively. Given our definition of ϵ, it can be shown using the calculation in (16) and Lemma 3.2 from [9], that $\tilde{\varphi}_b$ is a good approximation to ϕ_1 and, after shifting by $\mathbf{d}$, ϕ_2.

We assume that on $B_A(\mathbf{r}_1, \eta_0)$ and $B_A(\mathbf{r}_2, \eta_0)$ that the potential V is radially symmetric. Then the eigenvalue problem for $\tilde{\lambda}_b$ and $\tilde{\varphi}_b$ can be reduced to a one-dimensional problem of the form

$$-\partial_r^2\tilde{\varphi}_b - \frac{1}{r}\partial_r\tilde{\varphi}_b + \frac{1}{h^2}V(r)\tilde{\varphi}_b = \tilde{\lambda}_b\tilde{\varphi}_b, \tilde{\varphi}_b(R) = 0,$$

where R is the radius of a radially symmetric domain in the balls $B_A(\mathbf{r}_j, \eta_0)$. We assume that $R \gg h$.

A WKB method can be employed in order to obtain constructive approximations to the orbital functions. For $r \ll 1$ the potential is assumed to have the asymptotic form

$$V(r) \sim V_0 r^2 + \cdots.$$

For small r there is a maximally balanced *inner* equation. With $r = h^{1/2}x$, the inner equation takes the form

$$-\partial_x^2\tilde{\varphi}_b - \frac{1}{x}\partial_x\tilde{\varphi}_b + V_0x^2\tilde{\varphi}_b - E_0\tilde{\varphi}_b(x) = 0. \tag{19}$$

The solution of the inner Equation (19) is

$$\tilde{\varphi}_b(r) = Ce^{-\sqrt{V_0}r^2/2h} \text{ with } E_0 = 2\sqrt{V_0},$$

where C is constant.

In the *middle* region, $0 < r \ll R$, there is a WKB solution of the form

$$\tilde{\varphi}_b = e^{\Pi_0(r)/h + \Pi_1(r) + \cdots}$$

which matches to the inner solution; we find

$$\tilde{\varphi}_b(r) \sim C_W \frac{1}{r^{1/2}(V(r))^{1/4}} e^{\theta(r)},$$

where $\theta(r)$ is given by

$$\theta(r) = \frac{1}{h}\int_r^R \sqrt{V(s)}ds - \frac{E_0}{2}\int_r^R \frac{ds}{\sqrt{V(s)}},$$

and C_W is a constant that appropriately matches to the inner solution with constant C.

To satisfy the boundary condition, we must also introduce a boundary layer near $r = R$. In the region $R - h \ll r \leq R$, the solution that matches to the exterior of the layer is given by

$$\tilde{\varphi}_b(r) \sim C_B \frac{1}{R^{1/2}(V(R))^{1/4}} \sinh\left(\frac{\sqrt{V(R)}}{h}(R - r)\right),$$

where C_B is a constant that appropriately matches, apart from exponentially small terms, to the previous solution with constant C_W.

Therefore we have constructed an explicit approximation to the orbital functions. This allows us to write tight-binding approximations in concrete terms and compute all integrals in the approximation for u_{hc} used in Theorem 6. The method works for other non-simple lattice problems as well.

Acknowledgments

This research was partially supported by the U.S. Air Force Office of Scientific Research, under grant FA9550-09-1-0250 and by NSF under grant DMS-0905779.

References

1. Y. S. Kivshar and G. P. Agrawal, *Optical Solitons: From Fibers to Photonic Crystals*, Academic Press, New York, NY, 2003.
2. N. W. Ashcroft and N. D. Merman, *Solid State Physics*, Holt, Rinehart, and Winston, New York, NY, 1976.
3. C. Kittel, *Quantum Theory of Solids*, J. Wiley and Sons, New York, NY, 1963.
4. P. R. Wallace, The band theory of graphite, *Phys. Rev.* 71:622–634 (1947).
5. C. J. Pethick and H. Smith, *Bose-Einstein Condensation in Dilute Gases*, Oxford University Press, Oxford, UK, 2008.
6. M. J. Ablowitz and Y. Zhu, Unified description of the dynamics of wave envelopes in two-dimensional simple periodic lattices, preprint (2011).
7. M. J. Ablowitz and Y. Zhu, Evolution of Bloch-mode envelopes in two-dimensional generalized honeycomb lattices, *Phys. Rev. A* 82:013840 (2010).
8. M. Reed and B. Simon, *Methods of Mathematical Physics IV: Analysis of Operators*, Academic Press, New York, NY, 1978.
9. A. Outassourt, Comportement semi-classique pour l'opérateur de Schrödinger à potentiel périodique, *J. Funct. Anal.* 72:65–93 (1987).
10. M. J. Ablowitz and Z. H. Musslimani, Discrete vector spatial solitons in a nonlinear waveguide array, *Phys. Rev. E* 65:056618 (2002).
11. D. N. Christodoulides and R. I. Joseph, Discrete self-focusing in nonlinear arrays of coupled waveguides, *Opt. Lett.* 13:794–796 (1988).
12. J. W. Fleischer, T. Carmon, M. Segev, N. K. Efremidis, and D. N. Christodoulides, Observation of discrete solitons in optically-induced real time waveguide arrays, *Phys. Rev. Lett.* 90:023902 (2003).
13. P. G. Kevrekidis, B. A. Malomed, and Y. B. Gaididei, Solitons in triangular and honeycomb dynamical lattices with the cubic nonlinearity, *Phys. Rev. E* 66:016609 (2002).
14. D. N. Neshev, T. J. Alexander, E. A. Ostrovskaya, Y. S. Kivshar, I. Martin, H. Makasyuk, and Z. G. Chen, Observation of discrete vortex solitons in optically induced photonic lattices, *Phys. Rev. Lett.* 92:123903 (2004).
15. J. K. Yang, I. Makasyuk, A. Bezryadina, and Z. Chen, Dipole and quadrupole solitons in optically-induced two-dimensional photonic lattices: Theory and experiment, *Opt. Lett.* 29:1662 (2004).

16. D. Pelinovsky and G. Schneider, Bounds on the tight-binding approximation for the Gross-Pitaevskii equation with a periodic potential, *J. Diff. Eq.* 248:837–849 (2010).
17. D. Pelinovsky, G. Schneider, and R. S. MacKay, Justification of the lattice equation for a nonlinear elliptic problem with a periodic potential, *Commun. Math. Phys.* 284:803–831 (2008).
18. C. Brouder, G. Panati, M. Calandra, C. Mourougane, and N. Marzari, Exponential localization of Wannier functions in insulators, *Phys. Rev. Lett.* 98:046402 (2007).
19. G. Panati, Triviality of Bloch and Bloch-Dirac bundles, *Ann. Henri Poincaré* 8:995–1011 (2007).
20. P. D. Hislop and I. M. Sigal, *Introduction to Spectral Theory with Applications to Schrödinger Operators*, Springer, New York, NY, 1996.
21. M. Dimassi and J. Sjöstrand, *Spectral Asymptotics in the Semi-Classical Limit*, Cambridge University Press, Cambridge, 1999.
22. B. Helffer, *Semi-Classical Analysis for the Schrödinger Operator and Applications*, Springer, Berlin, 1988.
23. L. C. Evans, *Partial Differential Equations*, AMS, Providence, R.I., 1998.

University of Colorado
Tsinghua University

(Received May 12, 2012)