

DEFECT MODES AND HOMOGENIZATION OF PERIODIC SCHRÖDINGER OPERATORS*

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Abstract. We consider the discrete eigenvalues of the operator $H_\varepsilon = -\Delta + V(\mathbf{x}) + \varepsilon^2 Q(\varepsilon\mathbf{x})$, where $V(\mathbf{x})$ is periodic and $Q(\mathbf{y})$ is localized on \mathbb{R}^d , $d \geq 1$. For $\varepsilon > 0$ and sufficiently small, discrete eigenvalues may bifurcate (emerge) from spectral band edges of the periodic Schrödinger operator, $H_0 = -\Delta_{\mathbf{x}} + V(\mathbf{x})$, into spectral gaps. The nature of the bifurcation depends on the homogenized Schrödinger operator $L_{A,Q} = -\nabla_{\mathbf{y}} \cdot A \nabla_{\mathbf{y}} + Q(\mathbf{y})$. Here, A denotes the inverse effective mass matrix, associated with the spectral band edge, which is the site of the bifurcation.

Key words. multiple scales, Lyapunov–Schmidt reduction, eigenvalue bifurcation, spectral band edge

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1. Introduction and outline. Self-adjoint elliptic partial differential operators with periodic coefficients, e.g., the Schrödinger operator with a periodic potential, the time-harmonic Helmholtz equation with variable refractive index, and the time-harmonic Maxwell equations with variable dielectric and permeability tensors, play a central role in wave propagation problems in classical and quantum physics. The spectrum of such operators, characterized by the Floquet–Bloch theory [29, 20, 12], consists of the union of closed intervals (spectral bands). The eigenstates are *extended* (not localized) and form a complete set with respect to which any function in $L^2(\mathbb{R}^d)$ may be represented.

In many problems in fundamental and applied physics, periodic media are perturbed by spatially localized defects. These may appear as random imperfections in a media, e.g., a defect in a crystal, or, as in engineering applications, they may be introduced deliberately in order to influence wave propagation [4, 17]. Since the essential spectrum is unchanged by a sufficiently localized and smooth perturbation (Weyl’s theorem [29]), typical localized perturbations will only introduce eigenvalues in *spectral gaps* of the spectrum with associated localized *defect modes*.

This paper is concerned with a class of localized (defect) perturbations to a periodic Schrödinger operator of the form

$$H_\varepsilon = -\Delta_{\mathbf{x}} + V(\mathbf{x}) + \varepsilon^2 Q(\varepsilon\mathbf{x}),$$

where $V(\mathbf{x})$ is periodic on \mathbb{R}^d , $Q(\mathbf{y})$ decays as $|\mathbf{y}|$ tends to infinity, and ε is a small parameter.

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Our main result, Theorem 3.1, concerns the perturbed eigenvalue problem

$$(1.1) \quad H_\varepsilon u_\varepsilon = \mu_\varepsilon u_\varepsilon, \quad u_\varepsilon \in H^1(\mathbb{R}^d),$$

for ε positive and sufficiently small. See section 3 for hypotheses on the periodic potential, V , and the localized perturbation, Q .

For ε sufficiently small, we prove the bifurcation of discrete eigenvalues into the spectral gaps, associated with the unperturbed operator, $H_0 = -\Delta + V(\mathbf{x})$. For any given spectral band edge, we give detailed expansions with error estimates for the perturbed eigenvalues and corresponding localized eigenfunctions in terms of the eigenstates of a *homogenized* Schrödinger operator

$$(1.2) \quad L_{A,Q} = - \sum_{j,l=1}^d \frac{\partial}{\partial y_j} A_{jl} \frac{\partial}{\partial y_l} + Q(\mathbf{y}).$$

Here, A_{jl} denotes the *inverse effective mass matrix*, associated with the particular band edge from which the bifurcation occurs; see Theorem 3.1. A_{jl} , derivable by formal multiple scale expansion (see section 4), is expressible in terms of the band edge (Floquet–Bloch) eigenstate. It is proportional to the Hessian matrix $D^2 E_{b_*}(\mathbf{k}_*)$ of the band dispersion function, associated with $-\Delta + V(\mathbf{x})$, evaluated at the band edge $E_* = E_{b_*}(\mathbf{k}_*)$.

Referring to the schematics of Figures 1.1 and 1.2, we discuss our results.

- Suppose the inverse effective mass matrix, A , is positive definite and assume $L_{A,Q}$ has an eigenvalue, $e_{A,Q} < 0$. This occurs if $Q(\mathbf{y})$ is a “down-defect” (sufficiently “deep” in dimensions $d \geq 3$) as in Figure 1.1a. In this case, Theorem 3.1 asserts the existence of an eigenvalue at $E_* + \varepsilon^2 e_{A,Q} + \mathcal{O}(\varepsilon^3) < E_*$.
- Now suppose the inverse effective mass matrix, A , is negative definite and $L_{A,Q}$ has an eigenvalue, $e_{A,Q} > 0$. This occurs if $Q(\mathbf{y})$ is an “up-defect” (sufficiently “high” in dimensions $d \geq 3$) as in Figure 1.1b. In this case, Theorem 3.1 asserts the existence of an eigenvalue at $E_* + \varepsilon^2 e_{A,Q} + \mathcal{O}(\varepsilon^3) > E_*$.
- Figure 1.2 shows a more general band edge bifurcation when $L_{A,Q}$ has three eigenvalues $e_{A,Q}^{(1)} < e_{A,Q}^{(2)} < e_{A,Q}^{(3)}$, the largest of which is degenerate with multiplicity three. Theorem 3.1 asserts the existence of five ordered eigenvalues at $E_* + \varepsilon^2 e_{A,Q}^{(j)} + \mathcal{O}(\varepsilon^3)$, $j = 1, 2$, and $E_* + \varepsilon^2 e_{A,Q}^{(3)} + \varepsilon^3 \mu_3^{(k)} + \mathcal{O}(\varepsilon^4)$, $k = 1, 2, 3$.

1.1. Outline of the paper and overview of the proof. Section 2 summarizes the required spectral theory for Schrödinger operators with periodic potentials and introduces variants of the classical Sobolev space, $H^s(\mathbb{R}^d)$, which provide a natural functional analytic setting. Section 3 contains the hypotheses on V and Q and the statement of our main theorem, Theorem 3.1. In section 4 we present a *formal* multiple scale/homogenization expansion in which we systematically construct bifurcating eigenstates and eigenvalues to any prescribed order. In section 5 we prove Theorem 3.1. In particular, we study the equations governing the correction, Ψ^ε to the N -term multiple scale expansion.

To obtain error bounds of suitably high order in ε , we use a Lyapunov–Schmidt approach. Specifically, we decompose the error into Floquet–Bloch modes associated with energies lying near the spectral band edge, E_* , and those lying “far” from E_* : $\Psi^\varepsilon = \Psi_{\text{near}}^\varepsilon + \Psi_{\text{far}}^\varepsilon$. $\Psi_{\text{near}}^\varepsilon$ has the character of a wave-packet, spectrally supported on

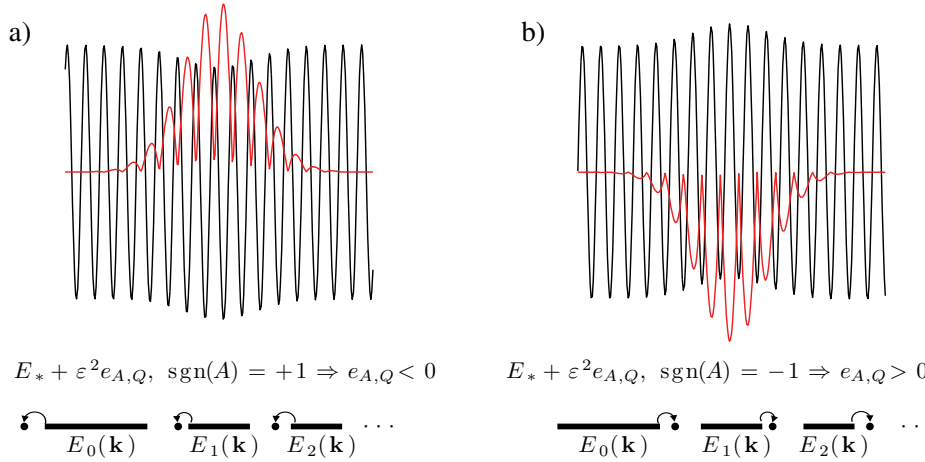


FIG. 1.1. (a) Periodic structure with “down-defect” and corresponding localized eigenstate for the case of positive definite effective mass tensor. (b) Periodic structure with “up-defect” and corresponding localized eigenstate for the case of negative definite effective mass tensor. Below the figures are shown eigenvalue bifurcations from band edges of the form $E_{b_*}(\mathbf{k}_*) = E_*$.

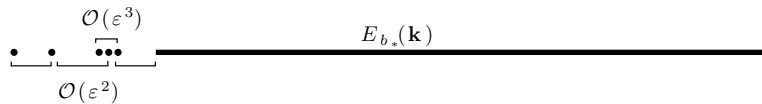


FIG. 1.2. Schematic of band edge bifurcations in the case where the inverse effective mass matrix, A , is positive definite. The homogenized operator, $L_{A,Q}$, is assumed to have two simple eigenvalues and one degenerate eigenvalue with multiplicity three.

a small interval with endpoint E_* . The next step is to solve for $\Psi_{\text{far}}^\varepsilon$ as a functional of the “parameter” $\Psi_{\text{near}}^\varepsilon$, with appropriate bounds. Substitution of $\Psi_{\text{far}}^\varepsilon[\Psi_{\text{near}}^\varepsilon]$ into the near equation implies a closed equation for $\Psi_{\text{near}}^\varepsilon$. With strong motivation from the structure of terms in the multiple scale expansion, we appropriately rescale, solve via the implicit function theorem, and estimate $\Psi_{\text{near}}^\varepsilon$. The approach we take has been applied in the context of the nonlinear Schrödinger/Pitaevskii equation in [31, 27, 10, 9, 16].

Previous work for linear Schrödinger operators. Bifurcation of eigenvalues from the edge of the continuous spectrum for Schrödinger operators with small decaying potentials, corresponding to weak defects in dimensions one and two for the case of a homogeneous medium or vacuum ($V \equiv 0$), was studied in [30]. Conditions ensuring the existence of eigenvalues in the gaps of periodic potentials were obtained in [1] and [13, 14], using the Birman–Schwinger (integral equation) formulation of the eigenvalue problem. Homogenization theory was applied to obtain eigenvalues in the spectral gaps of a class of periodic divergence form elliptic operators, governing localized states in high contrast media in [18, 8]. An elementary variational argument in spatial dimensions one and two, yielding general conditions for the existence of discrete modes in spectral gaps of periodic potentials, was recently presented in [26]. More general, variational methods can be applied to obtain defect modes which are obtained as infinite-dimensional saddle points of *strongly indefinite* functionals; see, for example, [11].

Our results concern a particular class of weak defects, slowly varying and of small amplitude: $\varepsilon^2 Q(\varepsilon \mathbf{x})$, which give rise to defect modes in any spatial dimension. We note that the one- and two-term truncated multiscale homogenization expansion of defect modes, which we construct, are natural trial functions for a variational proof of existence of ground states; see the discussion in Appendix B. Note also that the scaling of the perturbing potential, $\varepsilon^2 Q(\varepsilon \mathbf{x})$, also arises naturally in solitary standing wave (“soliton defect mode”) bifurcations from band edges of periodic potentials in the nonlinear Schrödinger/Gross–Pitaevskii equation [16].

Homogenization theory has been used to study periodic elliptic divergence form operators near spectral band edges in [6, 7, 2]. Homogenization results for the time-dependent Schrödinger equation with a scaling equivalent to the one considered here were obtained by two-scale convergence methods in [3]; see also [28, 5, 2]. In [3] the contrast between the scaling we use and the semiclassical scaling is discussed. These results establish the validity of the homogenized time-dependent Schrödinger equation on certain finite time scales. The results of the present paper focus on a subclass of solutions, bound states, which are controlled on infinite time scales.

Finally, we mention work on effective classical electron motion in solid state physics, derived from the Schrödinger equation for an electron in a spatially periodic Hamiltonian, perturbed by spatially slowly varying electrostatic and magnetic potentials [22, 24, 25], in a semiclassical limit.

1.2. Notation and conventions. We note that we may, without loss of generality, restrict ourselves to the case where the fundamental period cell is $\Omega = [0, 1]^d$. Indeed, let \mathcal{B} denote the fundamental period cell, spanned by the linearly independent vectors $\{\mathbf{r}_1, \dots, \mathbf{r}_d\}$ and define the constant matrix \mathcal{R}^{-1} to be the matrix whose j th column is \mathbf{r}_j . Then, under the change of coordinates $\mathbf{x} \mapsto \mathbf{z} = \mathcal{R}\mathbf{x}$,

$$\begin{aligned} & -\nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{x}} + V(\mathbf{x}) \text{ acting on } L^2_{\text{per}}(\mathcal{B}) \text{ transforms to} \\ & -\nabla_{\mathbf{z}} \cdot \alpha \nabla_{\mathbf{z}} + \tilde{V}(\mathbf{z}) \equiv - \sum_{i,j=1}^d \alpha_{ij} \frac{\partial^2}{\partial z_i \partial z_j} + \tilde{V}(\mathbf{z}) \\ & \text{acting on } L^2_{\text{per}}([0, 1]^d), \text{ where} \\ & \alpha = \mathcal{R}\mathcal{R}^T, \quad \tilde{V}(\mathbf{z}) = V(\mathcal{R}^{-1}\mathbf{z}), \quad \mathbf{x} = \mathcal{R}^{-1}\mathbf{z}. \end{aligned}$$

1. Integrals with unspecified region of integration are assumed to be taken over \mathbb{R}^d , i.e., $\int f = \int_{\mathbb{R}^d} f(\mathbf{x}) d\mathbf{x}$.
2. For $f, g \in L^2$, the Fourier transform and its inverse are given by

$$\begin{aligned} (1.3) \quad \mathcal{F}\{f\}(\mathbf{k}) &\equiv \hat{f}(\mathbf{k}) = \int e^{-2\pi i \mathbf{k} \cdot \mathbf{x}} f(\mathbf{x}) d\mathbf{x}, \\ \mathcal{F}^{-1}\{g\}(\mathbf{x}) &\equiv \check{g}(\mathbf{x}) = \int e^{2\pi i \mathbf{x} \cdot \mathbf{k}} g(\mathbf{k}) d\mathbf{k}. \end{aligned}$$

Thus, $\mathcal{F}\mathcal{F}^{-1} = \text{Id}$.

3. $\Omega = [0, 1]^d$ is the fundamental period cell; $\Omega^* = [-1/2, 1/2]^d$ is the dual fundamental cell or Brillouin zone.
4. $1_A(\mathbf{x})$ is the indicator function of the set A ; $\chi(|\mathbf{k}| \leq a) \equiv 1_{\{\mathbf{k} \in \Omega^* : |\mathbf{k}| \leq a\}}$.
5. The repeated index summation convention is used throughout.

6. Fourier spectral cutoff:

$$\chi(|\nabla| < a)G(\mathbf{x}) \equiv (\mathcal{F}^{-1}\chi(|\mathbf{k}| < a)\mathcal{F})G = \int e^{2\pi i\mathbf{x}\cdot\mathbf{k}}\chi(|\mathbf{k}| < a)\widehat{G}(\mathbf{k})d\mathbf{k}. \tag{1.4}$$

7. \mathcal{T} and \mathcal{T}^{-1} denote the Gel'fand–Bloch transform and its inverse; see section 2.

8. Bloch spectral cutoff:

$$\chi(|\nabla| < a)G(\mathbf{x}) \equiv \mathcal{T}^{-1} \left\{ \sum_{b \geq 0} \chi(|\cdot| < a\delta_{bb_*})\mathcal{T}_b \{G\}(\cdot) p_b(\mathbf{x}; \cdot) \right\}(\mathbf{x}),$$

where b_* is the index of the spectral band under consideration.

9. $H^s = H^s(\mathbb{R}^d)$ is the Sobolev space of order s :

$$\|f\|_{H^s}^2 \equiv \sum_{|\alpha| \leq s} \|\partial^\alpha f\|_{L^2}^2 \sim \|\widehat{f}\|_{L^{2,s}}^2 = \int_{\mathbb{R}^d} (1 + |\mathbf{k}|^{\frac{s}{2}})^2 |\widehat{f}(\mathbf{k})|^2 d\mathbf{k}. \tag{1.5}$$

2. Spectral theory for periodic potentials. In this section we summarize basic results on the spectral theory of Schrödinger operators with periodic potentials; see, for example, [29, 20, 12].

Gel'fand–Bloch transform. Given $f \in L^2(\mathbb{R}^d)$, we introduce the transform \mathcal{T} and its inverse as follows:

$$\mathcal{T}\{f(\cdot)\}(\mathbf{x}; \mathbf{k}) = \widetilde{f}(\mathbf{x}; \mathbf{k}) = \sum_{\mathbf{z} \in \mathbb{Z}^d} e^{2\pi i\mathbf{z}\cdot\mathbf{x}} \widehat{f}(\mathbf{k} + \mathbf{z}), \tag{2.1}$$

$$\mathcal{T}^{-1}\{\widetilde{f}(\mathbf{x}; \cdot)\}(\mathbf{x}) = \int_{\Omega^*} e^{2\pi i\mathbf{x}\cdot\mathbf{k}} \widetilde{f}(\mathbf{x}; \mathbf{k}) d\mathbf{k}. \tag{2.2}$$

One can check that $\mathcal{T}^{-1}\mathcal{T} = \text{Id}$.

Two important properties of the transformation \mathcal{T} are $\mathcal{T}\partial_{x_j}f = (\partial_{x_j} + 2\pi ik_j)\mathcal{T}f$ and $(\mathcal{T}e^{2\pi i\mathbf{k}\cdot}f)(\mathbf{x}, \mathbf{k}) = e^{2\pi i\mathbf{k}\cdot\mathbf{x}}\mathcal{T}f(\mathbf{x}, \mathbf{k})$. It follows that

$$(\mathcal{T}\Phi(\nabla)e^{2\pi i\mathbf{k}\cdot}f)(\mathbf{x}, \mathbf{k}) = e^{2\pi i\mathbf{k}\cdot\mathbf{x}}\Phi(\nabla + 2\pi i\mathbf{k})(\mathcal{T}f)(\mathbf{x}, \mathbf{k}), \tag{2.3}$$

$$\mathcal{T}(v(\cdot)f)(\mathbf{x}, \mathbf{k}) = v(\mathbf{x})(\mathcal{T}f)(\mathbf{x}, \mathbf{k}) \text{ if } v \text{ is periodic.} \tag{2.4}$$

Floquet–Bloch states. We seek solutions of the eigenvalue equation

$$(-\Delta + V(\mathbf{x}))u(\mathbf{x}) = Eu(\mathbf{x}) \tag{2.5}$$

in the form $u(\mathbf{x}; \mathbf{k}) = e^{2\pi i\mathbf{k}\cdot\mathbf{x}}p(\mathbf{x}; \mathbf{k})$, $\mathbf{k} \in \Omega^*$, where $p(\mathbf{x}; \mathbf{k})$ is periodic in \mathbf{x} with fundamental period cell Ω . $p(\mathbf{x}; \mathbf{k})$ then satisfies the periodic elliptic boundary value problem:

$$\left(-(\nabla + 2\pi i\mathbf{k})^2 + V(\mathbf{x})\right)p(\mathbf{x}; \mathbf{k}) = E(\mathbf{k})p(\mathbf{x}; \mathbf{k}), \quad \mathbf{x} \in \mathbb{T}^d. \tag{2.6}$$

For each $\mathbf{k} \in \Omega^*$, the eigenvalue problem (2.6) has a discrete set of eigenpairs $\{p_b(\mathbf{x}; \mathbf{k}), E_b(\mathbf{k})\}_{b \geq 0}$ which form a complete orthonormal set in $L^2_{\text{per}}(\Omega)$. The spectrum of $-\Delta + V(\mathbf{x})$ in $L^2(\mathbb{R}^d)$ is the union of closed intervals:

$$\text{spec}(-\Delta + V) = \bigcup_{b \geq 0, \mathbf{k} \in \Omega^*} E_b(\mathbf{k}). \tag{2.7}$$

We will study the bifurcation of eigenvalues from the band edge

$$(2.8) \quad E_* \equiv E_{b_*}(\mathbf{k}_*), \quad k_{*,j} \in \{0, 1/2\}, \quad j = 1, \dots, d,$$

with the associated, real-valued band edge eigenfunction

$$(2.9) \quad w(\mathbf{x}) \equiv e^{2\pi i \mathbf{k}_* \cdot \mathbf{x}} p_{b_*}(\mathbf{x}; \mathbf{k}_*) \in L^2(\Omega).$$

For example, the lowest band edge is $E_0(0)$ and the associated eigenfunction is periodic $p_0(\mathbf{x} + \mathbf{e}_j; 0) = p_0(\mathbf{x}; 0)$, $j = 1, \dots, d$, for the standard Cartesian basis vectors $\{\mathbf{e}_j\}_{j=1}^d$.

Remark 2.1. Since

$$(2.10) \quad w(\mathbf{x} + \mathbf{e}_j) = e^{2\pi i k_{*,j}} w(\mathbf{x}) = s_j w(\mathbf{x}),$$

where $s_j = +1$ if $k_{*,j} = 0$ and $s_j = -1$ otherwise, the natural function space in which to work is $L^2_{\text{symm}}(\Omega)$, i.e., $f \in L^2_{\text{symm}}(\Omega)$ if $f \in L^2(\Omega)$ and $f(\mathbf{x} + \mathbf{e}_j) = s_j f(\mathbf{x})$. Without loss of generality, and for ease of presentation, we focus on the case where $s_j = +1$, $j = 1, \dots, d$, so that $L^2_{\text{symm}}(\Omega) = L^2_{\text{per}}(\Omega)$, the space of square integrable, periodic functions. This implies that $\mathbf{k}_* = 0$. The more general case in (2.8) can be handled by taking $\mathbf{k} \rightarrow (\mathbf{k} - \mathbf{k}_*)$ and interpreting values of \mathbf{k} reflected about the boundary of Ω^* . The simplicity of E_* and the relation $\nabla E_{b_*}(\mathbf{k}_*) = 0$ (see hypothesis H2 in section 3) implies that $E(\mathbf{k}' + \mathbf{k}_*)$ can be extended as an even function of $k'_j = k_j - k_{j,*}$ for $j = 1, \dots, d$ [29].

We will make repeated use of the following self-adjoint operator:

$$(2.11) \quad L_* \equiv -\Delta + V(\mathbf{x}) - E_* : H^2_{\text{per}}(\Omega) \rightarrow L^2(\Omega).$$

Projections \mathcal{T}_b and completeness of Floquet–Bloch states. Define

$$(2.12) \quad \mathcal{T}_b\{f\}(\mathbf{k}) \equiv \langle p_b(\cdot; \mathbf{k}), \tilde{f}(\cdot; \mathbf{k}) \rangle_{L^2(\Omega)} \equiv \int_{\Omega} \overline{p_b(\mathbf{x}; \mathbf{k})} \tilde{f}(\mathbf{x}; \mathbf{k}) \, d\mathbf{x}.$$

By completeness of $\{p_b(\mathbf{x}; \mathbf{k})\}_{b \geq 0}$,

$$\tilde{f}(\mathbf{x}; \mathbf{k}) = \sum_{b \geq 0} \mathcal{T}_b\{f\}(\mathbf{k}) p_b(\mathbf{x}; \mathbf{k}).$$

Furthermore, applying \mathcal{T}^{-1} , we have

$$(2.13) \quad f(\mathbf{x}) = \sum_{b \geq 0} \int_{\Omega^*} \mathcal{T}_b\{f\}(\mathbf{k}) u_b(\mathbf{x}; \mathbf{k}) \, d\mathbf{k}$$

$$(2.14) \quad = \sum_{b \geq 0} \int_{\Omega^*} \langle u_b(\cdot; \mathbf{k}), f \rangle_{L^2(\mathbb{R}^d)} u_b(\mathbf{x}; \mathbf{k}) \, d\mathbf{k},$$

where $u_b(\mathbf{x}; \mathbf{k}) = e^{2\pi i \mathbf{k} \cdot \mathbf{x}} p_b(\mathbf{x}; \mathbf{k})$. The second equality follows from an application of the Poisson summation formula.

Sobolev spaces and the Gel'fand–Bloch transform. Recall the Sobolev space, H^s , the space of functions with square-integrable derivatives of order $\leq s$. Since $E_0(0) = \inf \text{spec}(-\Delta + V)$, then $L_0 = -\Delta + V(\mathbf{x}) - E_0(0)$ is a nonnegative operator and $H^s(\mathbb{R}^d)$ has the equivalent norm defined by

$$\|\phi\|_{H^s} \sim \|(I + L_0)^{\frac{s}{2}} \phi\|_{L^2}.$$

Introduce the space (see, e.g., [27, 9])

$$(2.15) \quad \mathcal{X}^s = L^2(\Omega^*, l^{2,s}),$$

with norm

$$(2.16) \quad \|\tilde{\phi}\|_{\mathcal{X}^s}^2 \equiv \int_{\Omega^*} \sum_{b=0}^{\infty} \left(1 + |b|^{\frac{2}{d}}\right)^s |\mathcal{T}_b\{\phi\}(\mathbf{k})|^2 d\mathbf{k}.$$

Now note that

$$(2.17) \quad \begin{aligned} \|\phi\|_{H^s}^2 &\sim \|(I + L_0)^{\frac{s}{2}} \phi\|_{L^2}^2 \\ &= \left\| \int_{\Omega^*} e^{2\pi i \mathbf{k} \cdot \cdot} \sum_{b \geq 0} \mathcal{T}_b\{\phi\}(\mathbf{k}) (1 + E_b(\mathbf{k}) - E_0(0))^{\frac{s}{2}} p_b(\cdot, \mathbf{k}) d\mathbf{k} \right\|_{L^2}^2 \\ &= \sum_{b \geq 0} \int_{\Omega^*} |\mathcal{T}_b\{\phi\}(\mathbf{k})|^2 |1 + E_b(\mathbf{k}) - E_0(0)|^s d\mathbf{k} \\ &\sim \sum_{b \geq 0} \left(1 + |b|^{\frac{2}{d}}\right)^s \int_{\Omega^*} |\mathcal{T}_b\{\phi\}(\mathbf{k})|^2 d\mathbf{k} \\ &\equiv \|\tilde{\phi}\|_{\mathcal{X}^s}^2. \end{aligned}$$

The second-to-last line follows from the Weyl asymptotics $E_b(\mathbf{k}) \sim b^{\frac{2}{d}}$ [15]. Thus we have the following proposition.

PROPOSITION 2.1. $H^s(\mathbb{R}^d)$ is isomorphic to \mathcal{X}^s for $s \geq 0$. Moreover, there exist positive constants C_1, C_2 such that for all $\phi \in H^s(\mathbb{R}^d)$

$$(2.18) \quad C_1 \|\phi\|_{H^s(\mathbb{R}^d)} \leq \|\tilde{\phi}\|_{\mathcal{X}^s} \leq C_2 \|\phi\|_{H^s(\mathbb{R}^d)}.$$

3. Main results. In this section we give a precise formulation of our main theorem, Theorem 3.1. The following are our assumptions.

H1. *Regularity.* $V \in L^\infty_{\text{per}}(\Omega)$, $Q \in H^\sigma(\mathbb{R}^d)$ for $\sigma > d$, $E_{b_*} \in C^3(\Omega^*)$, and $p_{b_*} \in L^2_{\text{per}}(\Omega; C^3(\Omega^*))$.

H2. *Band edge.* $E_* \equiv E_{b_*}(\mathbf{k}_*)$, where \mathbf{k}_* is an endpoint of the b_* th band such that

(a) E_* is a simple eigenvalue with corresponding eigenfunction

$$w(\mathbf{x}) \equiv e^{2\pi i \mathbf{k}_* \cdot \mathbf{x}} p_{b_*}(\mathbf{x}; \mathbf{k}_*) \in H^2_{\text{per}}(\Omega)$$

and normalization $\|w\|_{L^2(\Omega)} = 1$;

(b) $\nabla E_{b_*}(\mathbf{k}_*) = 0$;

(c) the Hessian matrix,

$$(3.1) \quad A \equiv \frac{1}{8\pi^2} D^2 E_{b_*}(\mathbf{k}_*),$$

is sign definite.

H3. *Existence of eigenvalue to homogenized equation.* Introduce the homogenized operator

$$(3.2) \quad L_{A,Q} \equiv -\nabla_{\mathbf{y}} \cdot A \nabla_{\mathbf{y}} + Q(\mathbf{y}) = -\sum_{j,l} \frac{\partial}{\partial y_j} A_{jl} \frac{\partial}{\partial y_l} + Q(\mathbf{y}).$$

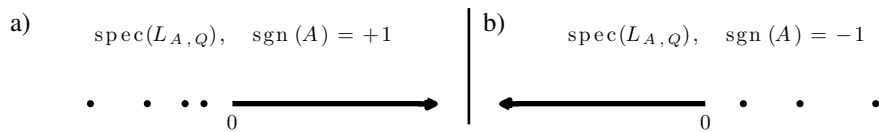


FIG. 3.1. Discrete and continuous spectrum of $L_{A,Q}$. (a) Positive definite effective mass tensor. (b) Negative definite effective mass tensor.

Set $\text{sgn}(A) = +1$ if A is positive definite and $\text{sgn}(A) = -1$ if A is negative definite. Assume $L_{A,Q}$ has a simple eigenvalue $e_{A,Q}$ with $\text{sgn}(A)e_{A,Q} < 0$ and corresponding eigenfunction $F_{A,Q}(\mathbf{y}) \in H^2(\mathbb{R}^d)$; i.e.,

$$(3.3) \quad L_{A,Q}F_{A,Q} = e_{A,Q}F_{A,Q}, \quad \int_{\mathbb{R}^d} F_{A,Q}^2(\mathbf{y})d\mathbf{y} = 1, \quad \text{sgn}(A)e_{A,Q} < 0;$$

see Figure 3.1a.

Remark 3.1. For further details regarding the smoothness properties of E_{b_*} and p_{b_*} with respect to \mathbf{k} , we refer the reader to [29, 32]. It can be verified that hypothesis H2 holds in one dimension at all band edges [12] and at the lowest band edge in arbitrary dimensions [19]. Band edges with multiplicity greater than one exist, e.g., for the separable potential $V(\mathbf{x}) = \sum_{j=1}^d V_1(x_j)$, $d \geq 2$.

THEOREM 3.1. (1) Positive definite effective mass tensor: Assume hypotheses H1–H3, with $\text{sgn}(A) = +1$. Then there exists $\varepsilon_0 > 0$ such that for all $0 < \varepsilon < \varepsilon_0$, (1.1) has an eigenpair μ_ε , $u_\varepsilon(\mathbf{x}; \mu_\varepsilon) \in H^2(\mathbb{R}^d)$. μ_ε lies in the spectral gap of $-\Delta + V(\mathbf{x})$ at a distance $\mathcal{O}(\varepsilon^2)$ below the spectral band edge having E_* as its left endpoint.

Moreover, to any order in ε , this solution can be approximated by the two-scale homogenization expansion (see (4.35), (5.1)), with error estimate

$$(3.4) \quad \left\| u_\varepsilon(\cdot; \mu_\varepsilon) - \sum_{n=0}^N \varepsilon^n U_n(\cdot, \varepsilon) \right\|_{H^2(\mathbb{R}^d)} \leq \varepsilon^{N-1}C,$$

$$\left| \mu_\varepsilon - E_* - \varepsilon^2 e_{A,Q} - \sum_{n=3}^N \varepsilon^n \mu_n \right| \leq \varepsilon^{N+1}C$$

for all $N \geq 4$ and some constant $C > 0$, which is independent of ε .

(2) Negative definite effective mass tensor: Assume hypotheses H1–H3, with $\text{sgn}(A) = -1$. Then the statement of part (1) applies, but now μ_ε lies in the spectral gap of $-\Delta + V(\mathbf{x})$ at a distance $\mathcal{O}(\varepsilon^2)$ above the spectral band edge having E_* as its right endpoint.

Theorem 3.1 extends to the case where $L_{A,Q}$ has multiple and/or degenerate eigenvalues with bifurcations from band edges with $\mathbf{k}_* \neq 0$, as discussed in the following remarks.

Remark 3.2 (general band edge bifurcations). As discussed in Remark 2.1, Theorem 3.1 generalizes to band edges where $\mathbf{k}_* \neq 0$, satisfying (2.8) so that $w(\mathbf{x}) \in L^2_{\text{symm}}(\Omega)$.

Remark 3.3 (multiple simple eigenvalues). Note that if $L_{A,Q}$ has M (finitely many) eigenvalues, $e_{A,Q}^{(j)}$, $j = 1, \dots, M$, of multiplicity one, then Theorem 3.1 applies directly. Specifically, there exists $\tilde{\varepsilon}_0 > 0$ such that for all $0 < \varepsilon < \tilde{\varepsilon}_0$, there are eigenvalue/eigenvector branches $\varepsilon \rightarrow (\mu_\varepsilon^{(j)}, u_\varepsilon(\cdot; \mu_\varepsilon^{(j)}))$. This behavior is shown in Figure 1.2 with two simple eigenvalue branches with spacings $\mathcal{O}(\varepsilon^2)$.

Remark 3.4 (branches emanating from degenerate eigenvalues of $L_{A,Q}$). In spatial dimensions, $d > 1$, the operator $L_{A,Q}$ may have degenerate eigenvalues, e.g., if there is symmetry in $Q(\mathbf{y})$. Suppose $e_{A,Q}$ has multiplicity M . Then, since $L_{A,Q}$ is self-adjoint, $e_{A,Q}$ perturbs, generically, to M distinct branches. Thus, applying the method of proof of Theorem 3.1, each degenerate eigenvalue of $L_{A,Q}$ of multiplicity M gives rise to M branches of eigenpairs of H_ε . The cluster of M distinct eigenvalues of H_ε is within an interval of size $\mathcal{O}(\varepsilon^3)$ about $E_* + \varepsilon^2 e_{A,Q}$. The j th eigenbranch satisfies the error estimates

$$(3.5) \quad \begin{aligned} & \left\| u_\varepsilon^{(j)}(\cdot; \mu_\varepsilon^{(j)}) - \sum_{n=0}^N \varepsilon^n U_n^{(j)}(\cdot, \varepsilon) \right\|_{H^2(\mathbb{R}^d)} \leq \varepsilon^{N-1} C, \\ & \left| \mu_\varepsilon^{(j)} - E_* - \varepsilon^2 e_{A,Q} - \sum_{n=3}^N \varepsilon^n \mu_n^{(j)} \right| \leq \varepsilon^{N+1} C \end{aligned}$$

for $j = 1, 2, \dots, M$, all $N \geq 4$, and some constant $C > 0$, which is independent of ε . This behavior is shown in Figure 1.2, where an eigenvalue of multiplicity three bifurcates from the band edge.

4. Homogenization and multiscale expansion. We derive a formal asymptotic expansion for the bound state that bifurcates from the band edge into a gap. The results of these calculations will be used as an ansatz in section 5 to rigorously prove existence and error estimates.

We assume that $u_\varepsilon(\mathbf{x}; \mu_\varepsilon)$ satisfies (1.1),

$$(4.1) \quad [-\Delta + V(\mathbf{x}) + \varepsilon^2 Q(\varepsilon \mathbf{x})] u_\varepsilon = \mu_\varepsilon u_\varepsilon,$$

and expand it in an asymptotic series as follows:

$$(4.2) \quad u_\varepsilon(\mathbf{x}; \mu_\varepsilon) = U_\varepsilon(\mathbf{x}, \mathbf{y}) = \sum_{n=0}^\infty \varepsilon^n U_n(\mathbf{x}, \mathbf{y}), \quad \mu_\varepsilon = E_* + \sum_{n=1}^\infty \varepsilon^n \mu_n,$$

where $\mathbf{y} = \varepsilon \mathbf{x}$ is the slow variable. Treating \mathbf{x} and \mathbf{y} as independent variables, (4.1) then takes the form

$$(4.3) \quad \left[-(\nabla_{\mathbf{x}} + \varepsilon \nabla_{\mathbf{y}})^2 + V(\mathbf{x}) + \varepsilon^2 Q(\mathbf{y}) \right] U_\varepsilon(\mathbf{x}, \mathbf{y}) = \mu_\varepsilon U_\varepsilon(\mathbf{x}, \mathbf{y}).$$

We seek a solution $U_\varepsilon(\mathbf{x}, \mathbf{y})$ which is periodic in the fast variable, \mathbf{x} , and localized in the slow variable, \mathbf{y} . Specifically, we assume $U_n(\mathbf{x}, \mathbf{y}) \in L^\infty_{\text{per}}(\Omega; H^2(\mathbb{R}^d))$. Inserting (4.2) and (4.3) into (4.1) and equating like powers of ε , we find

$$(4.4) \quad \mathcal{O}(\varepsilon^0) : \quad L_* U_0 \equiv [-\Delta_{\mathbf{x}} + V(\mathbf{x}) - E_*] U_0 = 0,$$

$$(4.5) \quad \mathcal{O}(\varepsilon^1) : \quad L_* U_1 = 2 \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{y}} U_0 + \mu_1 U_0,$$

$$(4.6) \quad \mathcal{O}(\varepsilon^2) : \quad L_* U_2 = 2 \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{y}} U_1 + \mu_1 U_1 - [-\Delta_{\mathbf{y}} + Q(\mathbf{y}) - \mu_2] U_0,$$

⋮

$$(4.7) \quad \mathcal{O}(\varepsilon^n) : \quad L_* U_n = 2 \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{y}} U_{n-1} + \mu_1 U_{n-1} - [-\Delta_{\mathbf{y}} + Q(\mathbf{y}) - \mu_2] U_{n-2} \\ + \sum_{j=3}^{n-1} \mu_j U_{n-j} + \mu_n U_0, \quad n \geq 3,$$

⋮

Viewed as a system of partial differential equations for functions of the fast variable \mathbf{x} , depending on a parameter \mathbf{y} , each equation in this hierarchy is of the form $L_*U = \mathcal{G}(\mathbf{x})$, where $\mathcal{G}(\mathbf{x})$ has the same symmetry as $w(\mathbf{x})$, the band edge state (see (2.9)), with period cell Ω . To solve these equations, we make repeated use of the following two solvability criteria based on the Fredholm alternative applied to the self-adjoint operators L_* and $L_{A,Q}$ with $\ker(L_*) = \text{span}\{w\} \subset L^2_{\text{per}}(\Omega)$ and $\ker(L_{A,Q}) = \text{span}\{F_{A,Q}\} \subset L^2(\mathbb{R}^d_{\mathbf{y}})$, respectively.

PROPOSITION 4.1. *Let $\mathcal{G} \in L^2_{\text{per}}(\Omega)$; then $L_*U = \mathcal{G}$ has an $H^2_{\text{per}}(\Omega)$ solution if and only if*

$$(4.8) \quad \langle w, \mathcal{G} \rangle_{L^2(\Omega)} = 0.$$

Remark 4.1. If $\mathbf{k}_* \neq 0$, then $L^2_{\text{per}}(\Omega)$ and $H^2_{\text{per}}(\Omega)$ are replaced by function spaces with the same symmetry as $w(\mathbf{x})$, $L^2_{\text{symm}}(\Omega)$ and $H^2_{\text{symm}}(\Omega)$. See Remark 2.1.

PROPOSITION 4.2. *Let $\mathcal{H} \in L^2(\mathbb{R}^d)$; then $L_{A,Q}F = \mathcal{H}$ has a solution $F \in H^2(\mathbb{R}^d_{\mathbf{y}})$ if and only if*

$$(4.9) \quad \langle F_{A,Q}, \mathcal{H} \rangle_{L^2(\mathbb{R}^d)} = 0.$$

4.1. $\mathcal{O}(\varepsilon^0)$ equation. From H2, there exist a unique, real, bounded eigenfunction $w \in H^2_{\text{per}}(\Omega)$ and a simple eigenvalue E_* that satisfy

$$(4.10) \quad L_*w = [-\Delta_{\mathbf{x}} + V(\mathbf{x}) - E_*]w = 0, \quad \|w\|_{L^2(\Omega)} = 1,$$

so that the general solution to (4.4) has the multiscale representation

$$(4.11) \quad U_0(\mathbf{x}, \mathbf{y}) = w(\mathbf{x})F_0(\mathbf{y})$$

for some $F_0(\mathbf{y}) \in H^2(\mathbb{R}^d)$ that will be determined at higher order.

4.2. $\mathcal{O}(\varepsilon^1)$ equation. Applying Proposition 4.1 to (4.5) gives the solvability condition

$$(4.12) \quad 2\partial_{y_j}F_0 \langle w, \partial_{x_j}w \rangle_{L^2(\Omega)} + \mu_1F_0 = 0.$$

Since the integrand in the first term, being the derivative of the symmetric function $w^2/2$, integrates to zero,

$$(4.13) \quad \mu_1 = 0.$$

Therefore, the general solution for U_1 consists of a homogeneous and particular solution

$$(4.14) \quad U_1(\mathbf{x}, \mathbf{y}) = w(\mathbf{x})F_1(\mathbf{y}) + 2\partial_{y_j}F_0(\mathbf{y})L_*^{-1}\{\partial_{x_j}w\}(\mathbf{x}),$$

where $F_1 \in H^2(\mathbb{R}^d)$ is to be determined at higher order.

Remark 4.2. For $d = 1$, the general solution is

$$(4.15) \quad U_1(x, y) = w(x)F_1(y) + \partial_yF_0(y)w(x) \left(-x + \frac{\int_0^x \frac{dx'}{w(x')^2}}{\int_0^1 \frac{dx'}{w(x')^2}} \right).$$

4.3. $\mathcal{O}(\varepsilon^2)$ equation. Inserting the expressions (4.13) and (4.14) into (4.6) yields

$$(4.16) \quad L_*U_2 = 2\partial_{y_j}F_1\partial_{x_j}w - \mathcal{L}[F_0],$$

where the linear operator $\mathcal{L}[G]$ for $G \in H^2(\mathbb{R}^d)$ is

$$(4.17) \quad \begin{aligned} \mathcal{L}[G](\mathbf{x}, \mathbf{y}) &= -4\partial_{x_j}L_*^{-1}\{\partial_{x_l}w\}(\mathbf{x})\partial_{y_j}\partial_{y_l}G(\mathbf{y}) \\ &+ w(\mathbf{x})[-\Delta_{\mathbf{y}} + Q(\mathbf{y}) - \mu_2]G(\mathbf{y}). \end{aligned}$$

DEFINITION 4.3. Define the operator $L_{A,Q} : H^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ by

$$(4.18) \quad L_{A,Q}G(\mathbf{y}) \equiv \langle w(\cdot), \mathcal{L}[G](\cdot, \mathbf{y}) \rangle_{L^2(\Omega)} = [-\nabla_{\mathbf{y}} \cdot A\nabla_{\mathbf{y}} + Q(\mathbf{y}) - e_{A,Q}]G(\mathbf{y}),$$

where $e_{A,Q}$ is the simple eigenvalue associated with the eigenfunction $F_{A,Q}(\mathbf{y})$ in hypothesis H3 and

$$(4.19) \quad A_{jl} \equiv \delta_{jl} - 4 \langle \partial_{x_j}w, L_*^{-1}\{\partial_{x_l}w\} \rangle_{L^2(\Omega)}.$$

PROPOSITION 4.4.

$$(4.20) \quad A_{jl} = \frac{1}{8\pi^2} \partial_{k_j} \partial_{k_l} E_{b_*}(\mathbf{k}_*).$$

We give the proof in Appendix A; see also [4].

Applying Proposition 4.1 to (4.16) gives

$$(4.21) \quad \langle w(\cdot), \mathcal{L}[F_0](\cdot, \mathbf{y}) \rangle_{L^2(\Omega)} = 0 \Leftrightarrow L_{A,Q}F_0 = 0, \quad \mu_2 = e_{A,Q},$$

which is the effective, homogenized equation for (1.1) with the effective mass tensor A . We have assumed in H3 the existence of the eigenpair $F_{A,Q} \in H^2(\mathbb{R}^d)$ and $e_{A,Q} \in \mathbb{R} \setminus \{0\}$. Thus, $F_0(\mathbf{y}) = F_{A,Q}(\mathbf{y})$.

The general solution for U_2 consists of a homogeneous and particular solution:

$$(4.22) \quad U_2(\mathbf{x}, \mathbf{y}) = w(\mathbf{x})F_2(\mathbf{y}) + 2\partial_{y_j}F_1(\mathbf{y})L_*^{-1}\{\partial_{x_j}w\}(\mathbf{x}) + L_*^{-1}\{\mathcal{L}[F_{A,Q}](\cdot, \mathbf{y})\}(\mathbf{x}).$$

4.4. $\mathcal{O}(\varepsilon^3)$ equation. Inserting (4.13), (4.14), and (4.22) into (4.7) with $n = 3$ gives

$$(4.23) \quad L_*U_3 = 2\partial_{y_j}F_2\partial_{x_j}w - \mathcal{L}[F_1] - \mathcal{H}_3 + \mu_3wF_{A,Q},$$

where \mathcal{H}_3 is known:

$$(4.24) \quad \begin{aligned} \mathcal{H}_3(\mathbf{x}, \mathbf{y}) &= -2\partial_{x_j}\partial_{y_j}L_*^{-1}\{\mathcal{L}[F_{A,Q}](\cdot, \mathbf{y})\}(\mathbf{x}) \\ &+ 2L_*^{-1}\{\partial_{x_j}w\}(\mathbf{x})[-\Delta_{\mathbf{y}} + Q(\mathbf{y}) - e_{A,Q}]\partial_{y_j}F(\mathbf{y}). \end{aligned}$$

By Proposition 4.1, (4.23) is solvable if and only if

$$(4.25) \quad L_{A,Q}F_1 = -\langle w(\cdot), \mathcal{H}_3(\cdot, \mathbf{y}) \rangle_{L^2(\Omega)} + \mu_3F_{A,Q}.$$

By Proposition 4.2, (4.25) has a solution if and only if

$$(4.26) \quad \mu_3 = \left\langle F_{A,Q}(\cdot), \langle w(\circ), \mathcal{H}_3(\circ, \cdot) \rangle_{L^2(\Omega)} \right\rangle_{L^2(\mathbb{R}^d)}.$$

We can now write F_1 in terms of $F_{A,Q}$ as

$$(4.27) \quad F_1(\mathbf{y}) = L_{A,Q}^{-1} \left\{ - \langle w(\circ), \mathcal{H}_3(\circ, \cdot) \rangle_{L^2(\Omega)} + \mu_3 F_{A,Q}(\cdot) \right\}(\mathbf{y}).$$

With this choice of F_1 , (4.23) is solvable and its general solution is

$$(4.28) \quad \begin{aligned} U_3(\mathbf{x}, \mathbf{y}) &= w(\mathbf{x})F_3(\mathbf{y}) + 2\partial_{y_j}F_2(\mathbf{y})L_*^{-1}\{\partial_{x_j}w\}(\mathbf{x}) \\ &\quad - L_*^{-1}\left\{\mathcal{L}[F_1](\cdot, \mathbf{y}) + \mathcal{H}_3(\cdot, \mathbf{y}) - \mu_3w(\cdot)F_{A,Q}(\mathbf{y})\right\}(\mathbf{x}), \end{aligned}$$

where $F_3(\mathbf{y})$ is to be determined. Note also that $F_2(\mathbf{y})$, introduced at $\mathcal{O}(\varepsilon^2)$, is to be determined.

4.5. (ε^n) order equation. Continuing the expansion to arbitrary $n \geq 4$ from (4.7), we have

$$(4.29) \quad L_*U_n = 2\partial_{y_j}F_{n-1}\partial_{x_j}w - \mathcal{L}[F_{n-2}] - \mathcal{H}_n + \mu_nwF_{A,Q},$$

where \mathcal{H}_n is completely determined by all the lower order solutions U_l , $l \leq n - 3$,

$$(4.30) \quad \begin{aligned} \mathcal{H}_n(\mathbf{x}, \mathbf{y}) &= 2\partial_{x_j}\partial_{y_j}L_*^{-1}\left\{\mathcal{L}[F_{n-3}](\cdot, \mathbf{y}) + \mathcal{H}_{n-1}(\cdot, \mathbf{y}) - \mu_{n-1}w(\cdot)F_{A,Q}(\mathbf{y})\right\}(\mathbf{x}) \\ &\quad - \sum_{l=3}^{n-1} \mu_l U_{n-l}. \end{aligned}$$

By Proposition 4.1, (4.29) is solvable if and only if

$$(4.31) \quad L_{A,Q}F_{n-2} = - \langle w(\cdot), \mathcal{H}_n(\cdot, \mathbf{y}) \rangle_{L^2(\Omega)} + \mu_nF_{A,Q}.$$

Furthermore, by Proposition 4.2, (4.31) is solvable if and only if

$$(4.32) \quad \mu_n = \left\langle F_{A,Q}(\cdot), \langle w(\circ), \mathcal{H}_n(\circ, \cdot) \rangle_{L^2(\Omega)} \right\rangle_{L^2(\mathbb{R}^d)}.$$

With this choice of μ_n , F_{n-2} is given by

$$(4.33) \quad F_{n-2}(\mathbf{y}) = L_{A,Q}^{-1} \left\{ - \langle w(\circ), \mathcal{H}_n(\circ, \cdot) \rangle_{L^2(\Omega)} + \mu_nF_{A,Q}(\cdot) \right\}(\mathbf{y}).$$

Finally, with this choice of F_{n-2} , $U_n(\mathbf{x}, \mathbf{y})$ is given by

$$(4.34) \quad \begin{aligned} U_n(\mathbf{x}, \mathbf{y}) &= w(\mathbf{x})F_n(\mathbf{y}) + 2\partial_{y_j}F_{n-1}(\mathbf{y})L_*^{-1}\{\partial_{x_j}w\}(\mathbf{x}) \\ &\quad - L_*^{-1}\left\{\mathcal{L}[F_{n-2}](\cdot, \mathbf{y}) + \mathcal{H}_n(\cdot, \mathbf{y}) - \mu_nw(\cdot)F_{A,Q}(\mathbf{y})\right\}(\mathbf{x}). \end{aligned}$$

Thus we have the following proposition.

PROPOSITION 4.5. *The first N equations (4.4), (4.5), (4.6), \dots , (4.7) are solvable with solutions $U_n(\mathbf{x}, \mathbf{y}) \in H_{per}^2(\Omega; H^2(\mathbb{R}^d))$, $n = 0, 1, \dots, N$, uniquely determined up to the two arbitrary slowly varying functions $F_N(\mathbf{y}), F_{N-1}(\mathbf{y}) \in H^2(\mathbb{R}^d)$ for $N \geq 1$. These functions are the slowly varying envelopes of the homogeneous solutions to the $N - 1$ th and N th order equations. Moreover,*

$$(4.35) \quad U_\varepsilon^{(N)}(\mathbf{x}, \mathbf{y}) \equiv \sum_{n=0}^N \varepsilon^n U_n(\mathbf{x}, \mathbf{y}), \quad \mu_\varepsilon^{(N)} \equiv E_* + \varepsilon^2 e_{A,Q} + \sum_{n=3}^N \varepsilon^n \mu_n,$$

with the particular choice $F_{n-1} = F_n \equiv 0$, is an approximate solution for the eigenvalue problem (4.1) (equivalently (1.1)) with error formally of order ε^{N+1} .

Remark 4.3. The multiscale form of the approximate eigenfunction given in Proposition 4.5 is used as a “trial function” in Appendix B to give a “quick” variational existence proof for defect modes bifurcating from the lowest band edge. We also show that a two-term approximation (leading order homogenized solution plus first nontrivial correction) yields a better estimate for the energy than the one-term approximation (leading order homogenized solution).

5. Proof of Theorem 3.1, bounds on $u(\cdot, \mu) - U_\varepsilon^{(N)}$, $\mu - \mu_\varepsilon^{(N)}$. To prove Theorem 3.1, we introduce the corrections $\Psi^\varepsilon(\mathbf{x})$ and Υ^ε to the approximate solution displayed in (4.35) through

$$(5.1) \quad u(\mathbf{x}; \mu) \equiv U_\varepsilon^{(N)}(\mathbf{x}, \varepsilon\mathbf{x}) + \varepsilon^{N-1}\Psi^\varepsilon(\mathbf{x}), \quad \mu \equiv \mu_\varepsilon^{(N)} + \varepsilon^{N+1}\Upsilon^\varepsilon.$$

Then the error Ψ^ε satisfies the equation

$$(5.2) \quad [L_* - \varepsilon^2 e_{A,Q} + \varepsilon^2 Q(\varepsilon\mathbf{x})]\Psi^\varepsilon(\mathbf{x}) = \varepsilon^2 R^\varepsilon[\Psi^\varepsilon, \Upsilon^\varepsilon](\mathbf{x}),$$

where

$$(5.3) \quad \begin{aligned} R^\varepsilon[\Psi^\varepsilon, \Upsilon^\varepsilon] &= \Upsilon^\varepsilon U_0 + 2\nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{y}} U_N - QU_{N-1} + \sum_{n=1}^N \mu_{n+1} U_{N-n} - \varepsilon QU_N \\ &\quad + \Psi^\varepsilon \left(\sum_{n=1}^{N-2} \varepsilon^n \mu_{n+2} + \varepsilon^{N-1} \Upsilon^\varepsilon \right) + \Upsilon^\varepsilon \sum_{n=1}^N \varepsilon^n U_n \\ &\quad + \sum_{n=1}^{N-1} \varepsilon^n \sum_{m=n}^N \mu_{m+1} U_{N+n-m} \\ &= \Upsilon^\varepsilon U_0 + 2\nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{y}} U_N - QU_{N-1} + \sum_{n=1}^N \mu_{n+1} U_{N-n} + \mathcal{O}(\varepsilon) \\ &\equiv \Upsilon^\varepsilon w_{F_{A,Q}} + U^\# + \mathcal{O}(\varepsilon), \\ U^\# &\equiv 2\nabla_x \cdot \nabla_y U_N = QU_{N-1} + \sum_{n=1}^N \mu_{n+1} U_{N-n}. \end{aligned}$$

The leading order multiscale approximation $U_0(\mathbf{x}, \varepsilon\mathbf{x}) = F_{A,Q}(\varepsilon\mathbf{x})w(\mathbf{x})$ in the ansatz (5.1) with $w(\mathbf{x}) = e^{2\pi i \mathbf{k}_* \cdot \mathbf{x}} p_{b_*}(\mathbf{x}; \mathbf{k}_*)$ being the band edge eigenfunction suggests that the dominant contribution to the frequency content of Ψ^ε will be near the band edge $E_* = E_{b_*}(\mathbf{k}_*)$. Therefore, it is natural to decompose Ψ^ε into Bloch eigenfunctions,

$$(5.4) \quad \Psi^\varepsilon(\mathbf{x}) = \sum_{b=0}^\infty \int_{\Omega^*} p_b(\mathbf{x}; \mathbf{k}) e^{2\pi i \mathbf{k} \cdot \mathbf{x}} \mathcal{T}_b\{\Psi^\varepsilon\}(\mathbf{k}) d\mathbf{k},$$

with associated energies or frequencies $E_b(\mathbf{k})$, where \mathbf{k} varies in the Brillouin zone Ω^* . Moreover, we introduce a spectral localization of Ψ^ε into frequencies “near” the band

edge and “far” from the band edge:

$$\begin{aligned}
 \Psi^\varepsilon(\mathbf{x}) &= \Psi_{\text{near}}^\varepsilon(\mathbf{x}) + \Psi_{\text{far}}^\varepsilon(\mathbf{x}) = \mathcal{T}^{-1} \tilde{\Psi}_{\text{near}}^\varepsilon(\mathbf{x}; \cdot) + \mathcal{T}^{-1} \tilde{\Psi}_{\text{far}}^\varepsilon(\mathbf{x}; \cdot), \\
 \tilde{\Psi}_{\text{near}}^\varepsilon(\mathbf{x}; \mathbf{k}) &= \Pi_{\text{near}} \Psi^\varepsilon(\mathbf{x}) \equiv \chi(|\mathbf{k} - \mathbf{k}_*| < \varepsilon^r) \mathcal{T}_{b_*} \{ \Psi^\varepsilon \}(\mathbf{k}) p_{b_*}(\mathbf{x}; \mathbf{k}), \\
 \tilde{\Psi}_{\text{far}}^\varepsilon(\mathbf{x}; \mathbf{k}) &= \Pi_{\text{far}} \Psi^\varepsilon(\mathbf{x}) \equiv \sum_{b=0}^\infty \chi(|\mathbf{k} - \mathbf{k}_*| \geq \varepsilon^r \delta_{b_*, b}) \mathcal{T}_b \{ \Psi^\varepsilon \}(\mathbf{k}) p_b(\mathbf{x}; \mathbf{k}),
 \end{aligned}
 \tag{5.5}$$

where $\delta_{n,m}$ is the Kronecker delta function and the indicator functions are defined as

$$\chi(|\mathbf{k} - \mathbf{k}_*| < \varepsilon^r) \equiv 1_{\{\mathbf{k} \in \Omega^* : |\mathbf{k} - \mathbf{k}_*| < \varepsilon^r\}}(\mathbf{k}), \quad \chi(|\mathbf{k} - \mathbf{k}_*| \geq \varepsilon^r) \equiv 1_{\{\mathbf{k} \in \Omega^* : |\mathbf{k} - \mathbf{k}_*| \geq \varepsilon^r\}}(\mathbf{k}).
 \tag{5.6}$$

Remark 5.1. For our analysis near the band edge, we will use Taylor expansions of various quantities about $\mathbf{k} = \mathbf{k}_*$. Without loss of generality, we will assume that $\mathbf{k}_* \equiv 0$, which enables a notationally cleaner presentation. See Remark 2.1.

We will use the conventions

$$\begin{aligned}
 \tilde{\Psi}_{\text{near}}^\varepsilon(\mathbf{k}) &\equiv \left\langle p_{b_*}(\cdot; \mathbf{k}), \tilde{\Psi}_{\text{near}}^\varepsilon(\cdot; \mathbf{k}) \right\rangle_{L^2(\Omega)}, \\
 \tilde{\Psi}_{\text{far}}^\varepsilon(\mathbf{k}) &\equiv \left(\left\langle p_b(\cdot; \mathbf{k}), \tilde{\Psi}_{\text{far}}^\varepsilon(\cdot; \mathbf{k}) \right\rangle_{L^2(\Omega)} \right)_{b \geq 0},
 \end{aligned}
 \tag{5.7}$$

where $\tilde{\Psi}_{\text{near}}^\varepsilon(\mathbf{k})$ is a scalar and $\tilde{\Psi}_{\text{far}}^\varepsilon(\mathbf{k})$ is an infinite vector. This decomposition was used in [10, 9, 16]. The parameter r is assumed to lie in the interval

$$r \in (2/3, 1),
 \tag{5.8}$$

the choice of which will be made clear later.

We now apply the Bloch transform to (5.2), project onto the Bloch modes $p_b(\cdot; \mathbf{k})$, and use the properties (2.3) and (2.4) to find

$$\begin{aligned}
 &[E_b(\mathbf{k}) - E_* - \varepsilon^2 e_{A,Q}] \mathcal{T}_b \{ \Psi^\varepsilon \}(\mathbf{k}) + \varepsilon^2 \mathcal{T}_b \{ Q(\varepsilon) \Psi^\varepsilon(\cdot) \}(\mathbf{k}) \\
 &= \varepsilon^2 \mathcal{T}_b \{ R^\varepsilon[\Psi^\varepsilon, \Upsilon^\varepsilon] \}(\mathbf{k}), \quad b = 0, 1, \dots
 \end{aligned}
 \tag{5.9}$$

We view this as a coupled system of equations for the near and far frequency components $\tilde{\Psi}_{\text{near}}^\varepsilon(\mathbf{k})$ and $\tilde{\Psi}_{\text{far}}^\varepsilon(\mathbf{k})$, $\mathbf{k} \in \Omega^*$:

$$\begin{aligned}
 \text{near:} & \begin{cases} (E_{b_*}(\mathbf{k}) - E_* - \varepsilon^2 e_{A,Q}) \tilde{\Psi}_{\text{near}}^\varepsilon(\mathbf{k}) \\ + \varepsilon^2 \chi(|\mathbf{k}| < \varepsilon^r) \mathcal{T}_{b_*} \{ Q(\varepsilon) \Psi_{\text{near}}^\varepsilon(\cdot) \}(\mathbf{k}) \\ = \varepsilon^2 \chi(|\mathbf{k}| < \varepsilon^r) \left[- \mathcal{T}_{b_*} \{ Q(\varepsilon) \Psi_{\text{far}}^\varepsilon(\cdot) \}(\mathbf{k}) \right. \\ \left. + \mathcal{T}_{b_*} \{ R^\varepsilon[\Psi_{\text{near}}^\varepsilon + \Psi_{\text{far}}^\varepsilon, \Upsilon^\varepsilon] \}(\mathbf{k}) \right], \end{cases} \\
 \text{far:} & \begin{cases} (E_b(\mathbf{k}) - E_* - \varepsilon^2 e_{A,Q}) \chi(|\mathbf{k}| \geq \varepsilon^r \delta_{b_*, b}) \tilde{\Psi}_{\text{far}, b}^\varepsilon(\mathbf{k}) \\ + \varepsilon^2 \chi(|\mathbf{k}| \geq \varepsilon^r \delta_{b_*, b}) \mathcal{T}_b \{ Q(\varepsilon) \Psi_{\text{far}}^\varepsilon(\cdot) \}(\mathbf{k}) \\ = \varepsilon^2 \chi(|\mathbf{k}| \geq \varepsilon^r \delta_{b_*, b}) \left[- \mathcal{T}_b \{ Q(\varepsilon) \Psi_{\text{near}}^\varepsilon(\cdot) \}(\mathbf{k}) \right. \\ \left. + \mathcal{T}_b \{ R^\varepsilon[\Psi_{\text{near}}^\varepsilon + \Psi_{\text{far}}^\varepsilon, \Upsilon^\varepsilon] \}(\mathbf{k}) \right], \quad b = 0, 1, 2, \dots \end{cases}
 \end{aligned}
 \tag{5.10}$$

$$\begin{aligned}
 \text{far:} & \begin{cases} (E_b(\mathbf{k}) - E_* - \varepsilon^2 e_{A,Q}) \chi(|\mathbf{k}| \geq \varepsilon^r \delta_{b_*, b}) \tilde{\Psi}_{\text{far}, b}^\varepsilon(\mathbf{k}) \\ + \varepsilon^2 \chi(|\mathbf{k}| \geq \varepsilon^r \delta_{b_*, b}) \mathcal{T}_b \{ Q(\varepsilon) \Psi_{\text{far}}^\varepsilon(\cdot) \}(\mathbf{k}) \\ = \varepsilon^2 \chi(|\mathbf{k}| \geq \varepsilon^r \delta_{b_*, b}) \left[- \mathcal{T}_b \{ Q(\varepsilon) \Psi_{\text{near}}^\varepsilon(\cdot) \}(\mathbf{k}) \right. \\ \left. + \mathcal{T}_b \{ R^\varepsilon[\Psi_{\text{near}}^\varepsilon + \Psi_{\text{far}}^\varepsilon, \Upsilon^\varepsilon] \}(\mathbf{k}) \right], \quad b = 0, 1, 2, \dots \end{cases}
 \end{aligned}
 \tag{5.11}$$

5.1. Lyapunov–Schmidt reduction. In this section, we derive a functional representation of the far frequency components in terms of the near frequency components with an associated estimate. After insertion into the near frequency equation, a closed system is obtained.

We use the implicit function theorem to solve the far frequency equations. To this end, we observe the following inequalities due to the definiteness of the matrix $A_{jl} = \frac{1}{8\pi^2} \partial_{k_j} \partial_{k_l} E_{b_*}(0)$ (see hypothesis H2):

$$(5.12) \quad \begin{aligned} |E_{b_*}(\mathbf{k}) - E_* - \varepsilon^2 e_{A,Q}| &= |A_{jl} k_j k_l + \mathcal{O}(|\mathbf{k}|^3)| \geq C\varepsilon^{2r} > 0, \quad \varepsilon^{2r} \leq |\mathbf{k}|, \quad \mathbf{k} \in \Omega^*, \\ |E_b(\mathbf{k}) - E_* - \varepsilon^2 e_{A,Q}| &\geq C > 0, \quad |b - b_*| \geq 1. \end{aligned}$$

We now have the following existence result.

PROPOSITION 5.1. *There exists $\varepsilon_0 > 0$ such that for $0 < \varepsilon < \varepsilon_0$, there is a mapping $(\psi, v, \varepsilon) \rightarrow \tilde{\Psi}_{far}^\varepsilon[\psi, v], \tilde{\Psi}_{far}^\varepsilon : L^2(\mathbb{R}^d) \times \mathbb{R}_v \times \mathbb{R}_\varepsilon \rightarrow \mathcal{X}^2$ such that $\tilde{\Psi}_{far}^\varepsilon[\Psi_{near}^\varepsilon, \Upsilon^\varepsilon]$ is the unique solution to the far frequency (5.11). The mapping $\tilde{\Psi}_{far}^\varepsilon$ is C^1 with respect to ψ and v . The solution of (5.11) satisfies the estimate*

$$(5.13) \quad \begin{aligned} \|\Psi_{far}^\varepsilon[\Psi_{near}^\varepsilon, \Upsilon^\varepsilon]\|_{H^2(\mathbb{R}^d)} &\leq C \|\tilde{\Psi}_{far}^\varepsilon[\Psi_{near}^\varepsilon, \Upsilon^\varepsilon]\|_{\mathcal{X}^2} \\ &\leq C\varepsilon^{2-2r} (1 + \Upsilon^\varepsilon + (1 + \varepsilon^{N-1}\Upsilon^\varepsilon) \|\Psi_{near}^\varepsilon\|_{L^2(\mathbb{R}^d)}) \end{aligned}$$

for $0 < r < 1$.

Proof. Since (5.11) is supported on frequencies away from E_* , we can divide it by $E_b(\mathbf{k}) - E_* - \varepsilon^2 e_{A,Q}$. This suggests studying the equivalent equation $\tilde{G} = 0$, where \tilde{G} has components

$$(5.14) \quad \begin{aligned} \tilde{G}_b[\tilde{\phi}, \varepsilon, \psi, v](\mathbf{k}) &\equiv \chi(|\mathbf{k}| \geq \varepsilon^r \delta_{b_*,b}) \left\{ \tilde{\phi}_b(\mathbf{k}) + \varepsilon^2 [E_b(\mathbf{k}) - E_* - \varepsilon^2 e_{A,Q}]^{-1} \right. \\ &\times \left. \left[\mathcal{T}_b \{Q(\varepsilon \cdot) \phi(\cdot)\}(\mathbf{k}) + \mathcal{T}_b \{Q(\varepsilon \cdot) \psi(\cdot)\}(\mathbf{k}) - \mathcal{T}_b \{R[\psi + \phi, v]\}(\mathbf{k}) \right] \right\}, \quad b \geq 0. \end{aligned}$$

Any function $\tilde{\phi} \in \mathcal{X}^2$ satisfying $\tilde{G}[\tilde{\phi}, \varepsilon, \psi, v] = 0$ is a solution of the far equations (5.11) with $\psi = \Psi_{near}^\varepsilon, v = \Upsilon^\varepsilon$. \tilde{G} is a continuous map $\mathcal{X}^2 \times \mathbb{R} \times \mathbb{R} \rightarrow \mathcal{X}^0$ and C^1 with respect to ψ and v satisfying the estimate

$$(5.15) \quad \|\tilde{G}[\tilde{\phi}, \varepsilon, \psi, v]\|_{\mathcal{X}^0} \leq C[1 + v + (1 + \varepsilon^{N+1-2r}v) \|\tilde{\phi}\|_{\mathcal{X}^0} + \varepsilon^{2-2r}(1 + \varepsilon^{N-1}v) \|\psi\|_{L^2(\mathbb{R}^d)}] < \infty.$$

Note that

$$(5.16) \quad \tilde{G}[0, 0, \psi, v] = 0.$$

The proposition follows from the implicit function theorem [23] if we can show that $D_{\tilde{\phi}} \tilde{G}[0, 0, \psi, v]$ is invertible. We have

$$(5.17) \quad \begin{aligned} (D_{\tilde{\phi}} \tilde{G}[\tilde{\phi}, \varepsilon, \psi, v] \tilde{f})_b(\mathbf{k}) &= \chi(|\mathbf{k}| \geq \varepsilon^r \delta_{b_*,b}) \tilde{f}_b(\mathbf{k}) \\ &+ \varepsilon^2 \chi(|\mathbf{k}| \geq \varepsilon^r \delta_{b_*,b}) \frac{\mathcal{T}_b \{Q(\varepsilon \cdot) f(\cdot)\}(\mathbf{k}) - \tilde{f}_b(\mathbf{k}) \left(\sum_{l=1}^{N-2} \varepsilon^l \mu_{l+2} + \varepsilon^{N-1} v \right)}{E_b(\mathbf{k}) - E_* - \varepsilon^2 e_{A,Q}}. \end{aligned}$$

Therefore, $D_{\tilde{\varphi}}\tilde{G}[0, 0, \psi, v] = I$ is invertible. Note that we use the fact that $0 < r < 1$ to conclude that $\lim_{\varepsilon \rightarrow 0} \varepsilon^2 \chi(|\mathbf{k}| \geq \varepsilon^r \delta_{b_*, b})/[E_b(\mathbf{k}) - E_* - \varepsilon^2 e_{A, Q}] \equiv 0$. The implicit function theorem implies that there exists $\varepsilon_0 > 0$ and a unique $\tilde{\Psi}_{\text{far}}^\varepsilon[\Psi_{\text{near}}^\varepsilon, \Upsilon^\varepsilon] \in \mathcal{X}^2$ satisfying

$$(5.18) \quad \tilde{G} \left[\tilde{\Psi}_{\text{far}}^\varepsilon[\Psi_{\text{near}}^\varepsilon, \Upsilon^\varepsilon], \varepsilon, \Psi_{\text{near}}^\varepsilon, \Upsilon^\varepsilon \right] = 0$$

for $0 < \varepsilon < \varepsilon_0$.

Equation (5.18) is equivalent to

$$(5.19) \quad \left(\tilde{\Psi}_{\text{far}}^\varepsilon \right)_b(\mathbf{k}) = -\varepsilon^2 \frac{\mathcal{T}_b \left\{ \Pi_{\text{far}} \left[Q(\varepsilon \cdot) \Psi_{\text{far}}^\varepsilon(\cdot) - R^\varepsilon[\Psi_{\text{near}}^\varepsilon + \Psi_{\text{far}}^\varepsilon, \Upsilon^\varepsilon](\cdot) \right] \right\}(\mathbf{k})}{E_b(\mathbf{k}) - E_* - \varepsilon^2 e_{A, Q}}.$$

We now demonstrate the inequality in (5.13). Using (2.18), (5.11), and the invertibility of $L_* - \varepsilon^2 e_{A, Q}$, we obtain

$$(5.20) \quad \begin{aligned} \|\Psi_{\text{far}}^\varepsilon\|_{H^2(\mathbb{R}^d)} &\leq C \left\| \tilde{\Psi}_{\text{far}}^\varepsilon \right\|_{\mathcal{X}^2} \\ &= \varepsilon^2 C \left\| \frac{\chi(|\cdot| \geq \varepsilon^r \delta_{b_*, b}) \mathcal{T}_b \left\{ Q(\varepsilon \circ) \Psi_{\text{far}}^\varepsilon(\circ) - R^\varepsilon[\Psi_{\text{near}}^\varepsilon, \Upsilon^\varepsilon](\circ) \right\}(\cdot)}{E_b(\cdot) - E_* - \varepsilon^2 e_{A, Q}} \right\|_{\mathcal{X}^2} \\ &\leq \varepsilon^{2-2r} C \left\| \frac{(1 + b^{2/d}) \mathcal{T}_b \left\{ Q(\varepsilon \circ) \Psi_{\text{far}}^\varepsilon(\circ) - R^\varepsilon[\Psi_{\text{near}}^\varepsilon, \Upsilon^\varepsilon](\circ) \right\}(\cdot)}{1 + b^{2/d}} \right\|_{\mathcal{X}^0} \\ &\leq \varepsilon^{2-2r} C \|Q(\varepsilon \cdot) \Psi_{\text{far}}^\varepsilon(\cdot) - R^\varepsilon[\Psi_{\text{near}}^\varepsilon, \Upsilon^\varepsilon](\cdot)\|_{L^2(\mathbb{R}^d)} \\ &\leq \varepsilon^{2-2r} C \left[(1 + \varepsilon^{N-1} \Upsilon^\varepsilon) \left(\|\Psi_{\text{far}}^\varepsilon(\cdot)\|_{L^2(\mathbb{R}^d)} + \|\Psi_{\text{near}}^\varepsilon(\cdot)\|_{L^2(\mathbb{R}^d)} \right) + 1 + \Upsilon^\varepsilon \right], \end{aligned}$$

where the constants C are independent of ε . The third inequality results from the Weyl eigenvalue asymptotics [15] and the bound (5.12). The last inequality results from direct estimation of the error terms (5.3). With ε small enough so that $\varepsilon^{2-2r} C \leq 1/2$, we can subtract the term involving $\varepsilon^{2-2r} C \|\Psi_{\text{far}}^\varepsilon\|_{H^2(\mathbb{R}^d)}$ from both sides of the inequality and then divide by $1 - \varepsilon^{2-2r} C(1 + \varepsilon^{N-1} \Upsilon^\varepsilon)$ to obtain the desired estimate (5.13). \square

Remark 5.2. Note that we do not obtain smoothness of $\Psi_{\text{far}}^\varepsilon$ in ε . When applying the implicit function theorem in the above proof, we did not use any smoothness of the map \tilde{G} in ε . This is because of the sharp, ε -dependent cutoff function $\chi(|\mathbf{k}| \geq \varepsilon^r)$.

Remark 5.3. The estimate for $\Psi_{\text{far}}^\varepsilon \in H^2(\mathbb{R}^d)$ and $\Psi_{\text{near}}^\varepsilon \in L^2(\mathbb{R}^d)$ in (5.13) can also be proved for $\Psi_{\text{far}}^\varepsilon \in H^s(\mathbb{R}^d)$ and $\Psi_{\text{near}}^\varepsilon \in H^{s-2}(\mathbb{R}^d)$ for $s \geq 2$. The proof for the case $s \geq 3$ involves application of the operator $(I + L_*)^{s/2-1}$, which can be shown to be equivalent to the H^{s-2} norm, to (5.2) and necessitates further regularity conditions on the functions $V(\mathbf{x})$, $Q(\varepsilon \mathbf{x})$, and $U_n(\mathbf{x}, \varepsilon \mathbf{x})$, $n = 0, 1, \dots, N$.

5.2. Near frequency equation and its scaling. We now study the near frequency equation (5.10) with the aid of certain Taylor expansions for $|\mathbf{k}| < \varepsilon^r$, where we invoke our regularity hypothesis H1:

$$(5.21) \quad \begin{aligned} E_{b_*}(\mathbf{k}) &= E_* + \frac{1}{2} \partial_{k_j} \partial_{k_l} E_{b_*}(0) k_j k_l + \frac{1}{6} \partial_{k_j} \partial_{k_l} \partial_{k_m} E_{b_*}(\mathbf{k}') k_j k_l k_m \\ &= E_* + A_{jl} k_j k_l + \frac{1}{6} \partial_{k_j} \partial_{k_l} \partial_{k_m} E_{b_*}(\mathbf{k}') k_j k_l k_m, \end{aligned}$$

$$(5.22) \quad \begin{aligned} p_{b_*}(\mathbf{x}; \mathbf{k}) &= p_{b_*}(\mathbf{x}; 0) + \partial_{k_j} p_{b_*}(\mathbf{x}; \mathbf{k}'') k_j \\ &= w(\mathbf{x}) + \partial_{k_j} p_{b_*}(\mathbf{x}; \mathbf{k}'') k_j \end{aligned}$$

for some $|\mathbf{k}'(\mathbf{k})|, |\mathbf{k}''(\mathbf{k})| < \varepsilon^r$. Inserting these expansions into the near frequency equation (5.10), we have

$$(5.23) \quad [A_{jl}k_jk_l - \varepsilon^2 e_{A,Q}] \tilde{\Psi}_{\text{near}}^\varepsilon(\mathbf{k}) + \varepsilon^2 \chi(|\mathbf{k}| < \varepsilon^r) \mathcal{T}_{b_*} \{Q(\varepsilon \cdot) \Psi_{\text{near}}^\varepsilon(\cdot)\}(\mathbf{k}) = \varepsilon^2 \tilde{R}_{\text{near}}^\varepsilon[\Psi_{\text{near}}^\varepsilon, \Upsilon^\varepsilon](\mathbf{k}),$$

where

$$(5.24) \quad \begin{aligned} \tilde{R}_{\text{near}}^\varepsilon[\Psi_{\text{near}}^\varepsilon, \Upsilon^\varepsilon](\mathbf{k}) &\equiv \chi(|\mathbf{k}| < \varepsilon^r) \left[\mathcal{T}_{b_*} \{R^\varepsilon[\Psi_{\text{near}}^\varepsilon + \Psi_{\text{far}}^\varepsilon[\Psi_{\text{near}}^\varepsilon, \Upsilon^\varepsilon], \Upsilon^\varepsilon]\}(\mathbf{k}) \right. \\ &\quad - \mathcal{T}_{b_*} \{Q(\varepsilon \cdot) \Psi_{\text{far}}^\varepsilon[\Psi_{\text{near}}^\varepsilon, \Upsilon^\varepsilon](\cdot)\}(\mathbf{k}) \\ &\quad \left. - \frac{1}{6\varepsilon^2} k_j k_l k_m \partial_{k_j} \partial_{k_l} \partial_{k_m} e_{b_*}(\mathbf{k}') \tilde{\Psi}_{\text{near}}^\varepsilon(\mathbf{k}) \right] \\ &= \chi(|\mathbf{k}| < \varepsilon^r) \mathcal{T}_{b_*} \{ \Upsilon^\varepsilon w(\cdot) F_{A,Q}(\varepsilon \cdot) + U^\#(\cdot, \varepsilon \cdot) \}(\mathbf{k}) \\ &\quad + \mathcal{O}_{\mathcal{X}^2} \left[(\varepsilon + \varepsilon^{2-2r} + \varepsilon^{3r-2}) \|\tilde{\Psi}_{\text{near}}^\varepsilon\|_{\mathcal{X}^2} \right], \end{aligned}$$

where the leading order behavior comes from the definition of R^ε in (5.3). Recall that $U^\#$ is defined in (5.3). The terms proportional to ε^{3r-2} put a further restriction on the exponent r . In order to keep $\tilde{R}_{\text{near}}^\varepsilon$ order one, we require

$$(5.25) \quad 2/3 < r < 1.$$

In this case, the error term satisfies the estimate

$$(5.26) \quad \begin{aligned} &\left\| \tilde{R}_{\text{near}}^\varepsilon[\Psi_{\text{near}}^\varepsilon, \Upsilon^\varepsilon] \right\|_{\mathcal{X}^2} \\ &\leq C \left[1 + \Upsilon^\varepsilon + (\varepsilon + \varepsilon^{2-2r} + \varepsilon^{3r-2}) \|\tilde{\Psi}_{\text{near}}^\varepsilon\|_{\mathcal{X}^2} \right]. \end{aligned}$$

Equation (5.23) can be rewritten as

$$(5.27) \quad \begin{aligned} &\left[A_{jl} \frac{k_j}{\varepsilon} \frac{k_l}{\varepsilon} - e_{A,Q} \right] \tilde{\Psi}_{\text{near}}^\varepsilon(\mathbf{k}) \\ &+ \chi \left(\left| \frac{\mathbf{k}}{\varepsilon} \right| < \varepsilon^{r-1} \right) \mathcal{T}_{b_*} \{Q(\varepsilon \cdot) \Psi_{\text{near}}^\varepsilon(\cdot)\}(\mathbf{k}) = \tilde{R}_{\text{near}}^\varepsilon[\Psi_{\text{near}}^\varepsilon, \Upsilon^\varepsilon](\mathbf{k}), \end{aligned}$$

suggesting that we seek a solution of (5.23), (5.24) in the form

$$(5.28) \quad \begin{aligned} \tilde{\Psi}_{\text{near}}^\varepsilon(\mathbf{k}) &= \chi(|\mathbf{k}| < \varepsilon^r) \frac{1}{\varepsilon^d} \hat{\Phi} \left(\frac{\mathbf{k}}{\varepsilon} \right) = \chi \left(\frac{|\mathbf{k}|}{\varepsilon} < \varepsilon^{r-1} \right) \frac{1}{\varepsilon^d} \hat{\Phi} \left(\frac{\mathbf{k}}{\varepsilon} \right), \\ \Psi_{\text{near}}^\varepsilon(\mathbf{x}) &= \mathcal{T}^{-1} \left\{ \chi(|\cdot| < \varepsilon^r) \frac{1}{\varepsilon^d} \hat{\Phi} \left(\frac{\cdot}{\varepsilon} \right) p_{b_*}(\mathbf{x}; \cdot) \right\}(\mathbf{x}) \\ &= \mathcal{T}^{-1} \left\{ \chi \left(\frac{|\cdot|}{\varepsilon} < \varepsilon^{r-1} \right) \frac{1}{\varepsilon^d} \hat{\Phi} \left(\frac{\cdot}{\varepsilon} \right) p_{b_*}(\mathbf{x}; \cdot) \right\}(\mathbf{x}). \end{aligned}$$

In the next two lemmas, Lemmas 5.2 and 5.3, we express the terms of (5.27), which involve the Gel'fand–Bloch transform, in terms of the classical Fourier transform plus a remainder, estimated to be small in ε .

LEMMA 5.2.

(A) Assume $\tilde{\Psi}_{near}^\varepsilon(\mathbf{k})$ is given by (5.28). Then

$$\begin{aligned} & \left[A_{jl} \frac{k_j}{\varepsilon} \frac{k_l}{\varepsilon} - e_{A,Q} \right] \tilde{\Psi}_{near}^\varepsilon(\mathbf{k}) \\ &= \mathcal{F}_{\mathbf{y}} \left\{ (A_{jl} \partial_{y_j} \partial_{y_l} - e_{A,Q}) \chi(|\nabla| < \varepsilon^{r-1}) \Phi \right\} \left(\frac{\mathbf{k}}{\varepsilon} \right). \end{aligned}$$

(B)

(5.29)

$$\mathcal{T}_{b_*} \{ Q(\varepsilon \cdot) \Psi_{near}^\varepsilon(\cdot) \}(\mathbf{k}) = \frac{1}{\varepsilon^d} \mathcal{F}_{\mathbf{y}} \left\{ Q \chi(|\nabla| \leq \varepsilon^{r-1}) \Phi \right\} \left(\frac{\mathbf{k}}{\varepsilon} \right) + \mathcal{E}(\mathbf{k}),$$

where

$$(5.30) \quad \|\mathcal{E}\|_{L^2(\mathbb{R}^d)} \leq C\varepsilon^s \|Q\|_{H^s(\mathbb{R}^d)} \|\Phi\|_{L^2(\mathbb{R}^d)},$$

with $s > d$ and $0 < r < 1$.

Proof of Lemma 5.2. Recall the notation $\mathcal{F}f = \widehat{f}$ for the Fourier transform given by (1.3). By (5.28) since \mathbf{k} is localized near 0 we have, Taylor expanding $p_{b_*}(\mathbf{x}; \mathbf{k})$ about $\mathbf{k} = 0$,

$$\begin{aligned} \Psi_{near}^\varepsilon(\mathbf{x}) &= p_{b_*}(\mathbf{x}; 0) \mathcal{F}^{-1} \left\{ \chi(|\cdot| < \varepsilon^r) \frac{1}{\varepsilon^d} \widehat{\Phi} \left(\frac{\cdot}{\varepsilon} \right) \right\}(\mathbf{x}) + \mathcal{E}_1(\mathbf{x}) \\ &= p_{b_*}(\mathbf{x}; 0) \chi(|\nabla_{\mathbf{y}}| < \varepsilon^{r-1}) \Phi(\mathbf{y})|_{\mathbf{y}=\varepsilon\mathbf{x}} + \mathcal{E}_1(\mathbf{x}), \\ \|\mathcal{E}_1\|_{L^2(\mathbb{R}^d)} &\leq C\varepsilon^r \|\Phi\|_{L^2(\mathbb{R}^d)}, \quad C = C(\|\nabla_{\mathbf{k}} p_{b_*}\|_{L^\infty(\Omega \times \Omega^*)^d}). \end{aligned}$$

Since \mathcal{T} commutes with multiplication by a periodic function (see (2.4)) and since $p_{b_*}(\mathbf{x}; 0)$ is periodic,

$$(5.31) \quad \begin{aligned} & \mathcal{T}\{Q(\varepsilon \cdot) \Psi_{near}^\varepsilon(\cdot)\}(\mathbf{x}, \mathbf{k}) \\ &= p_{b_*}(\mathbf{x}; 0) \mathcal{T}\{Q(\varepsilon \cdot) \chi(|\nabla_{\varepsilon \cdot}| < \varepsilon^{r-1}) \Phi(\varepsilon \cdot)\}(\mathbf{x}, \mathbf{k}) + \mathcal{T}\{Q(\varepsilon \cdot) \mathcal{E}_1(\cdot)\}(\mathbf{x}, \mathbf{k}). \end{aligned}$$

By the definition of \mathcal{T} , (2.1), we have

$$(5.32) \quad \begin{aligned} & \mathcal{T}\{Q(\varepsilon \cdot) \chi(|\nabla_{\varepsilon \cdot}| < \varepsilon^{r-1}) \Phi(\varepsilon \cdot)\}(\mathbf{x}, \mathbf{k}) \\ &= \mathcal{F}_{\mathbf{x}} \left\{ Q(\varepsilon \cdot) \chi(|\nabla_{\varepsilon \cdot}| < \varepsilon^{r-1}) \Phi(\varepsilon \cdot) \right\}(\mathbf{k}) \\ &+ \sum_{\mathbf{m} \neq 0} \mathcal{F}_{\mathbf{x}} \left\{ Q(\varepsilon \cdot) \mathcal{F}_{\mathbf{k}}^{-1} \left\{ \chi(|\circ| < \varepsilon^r) \frac{1}{\varepsilon^d} \widehat{\Phi} \left(\frac{\circ}{\varepsilon} \right) \right\}(\cdot) \right\}(\mathbf{k} + \mathbf{m}) e^{2\pi i \mathbf{m} \cdot \mathbf{x}} \\ &= \frac{1}{\varepsilon^d} \mathcal{F}_{\mathbf{y}} \left\{ Q(\cdot) \chi(|\nabla| < \varepsilon^{r-1}) \Phi(\cdot) \right\} \left(\frac{\mathbf{k}}{\varepsilon} \right) \\ (5.33) \quad &+ \sum_{|\mathbf{m}| \geq 1} \int \widehat{Q} \left(\frac{\mathbf{l}}{\varepsilon} \right) \frac{1}{\varepsilon^d} \widehat{\Phi} \left(\frac{\mathbf{k} + \mathbf{m} - \mathbf{l}}{\varepsilon} \right) \chi(|\mathbf{k} + \mathbf{m} - \mathbf{l}| < \varepsilon^r) d\mathbf{l} e^{2\pi i \mathbf{m} \cdot \mathbf{x}}. \end{aligned}$$

To prove (5.30) we need to estimate the sum in (5.33) for $|\mathbf{k}| < \varepsilon^r$. For such \mathbf{k}

the sum can be estimated as follows:

$$\begin{aligned}
 & \sum_{|\mathbf{m}| \geq 1} \int \left| \widehat{Q} \left(\frac{\mathbf{l}}{\varepsilon} \right) \right| \frac{1}{\varepsilon^d} \left| \widehat{\Phi} \left(\frac{\mathbf{k} + \mathbf{m} - \mathbf{l}}{\varepsilon} \right) \right| \chi(|\mathbf{k} + \mathbf{m} - \mathbf{l}| < \varepsilon^r) \, d\mathbf{l} \\
 & \leq \sum_{|\mathbf{m}| \geq 1} \left(\int_{|\mathbf{m}-\mathbf{l}| \leq 2\varepsilon^r} \left| \widehat{Q} \left(\frac{\mathbf{l}}{\varepsilon} \right) \right|^2 \frac{1}{\varepsilon^d} \, d\mathbf{l} \right)^{\frac{1}{2}} \left(\int_{|\mathbf{m}-\mathbf{l}| \leq 2\varepsilon^r} \left| \widehat{\Phi} \left(\frac{\mathbf{l}}{\varepsilon} \right) \right|^2 \frac{1}{\varepsilon^d} \, d\mathbf{l} \right)^{\frac{1}{2}} \\
 & \leq C \sum_{|\mathbf{m}| \geq 1} \left(1 + \left| \frac{\mathbf{m}}{\varepsilon} \right|^2 \right)^{-\frac{s}{2}} \left(\int_{|\mathbf{m}-\mathbf{l}| \leq 2\varepsilon^r} \left| \widehat{Q} \left(\frac{\mathbf{l}}{\varepsilon} \right) \right|^2 \left(1 + \left| \frac{\mathbf{l}}{\varepsilon} \right|^2 \right)^s \frac{1}{\varepsilon^d} \, d\mathbf{l} \right)^{\frac{1}{2}} \|\Phi\|_{L^2(\mathbb{R}^d)} \\
 & \leq C \varepsilon^s \sum_{|\mathbf{m}| \geq 1} |\mathbf{m}|^{-s} \|Q\|_{H^s(\mathbb{R}^d)} \|\Phi\|_{L^2(\mathbb{R}^d)} \leq C \varepsilon^s \|Q\|_{H^s(\mathbb{R}^d)} \|\Phi\|_{L^2(\mathbb{R}^d)}, \quad s > d.
 \end{aligned}
 \tag{5.34}$$

A similar calculation shows

$$\|\mathcal{T}\{Q(\varepsilon \cdot) \mathcal{E}_1(\cdot)\}\|_{L^2(\mathbb{R}^d, \Omega^*)} \leq C \varepsilon^{s+r} \|Q\|_{H^s(\mathbb{R}^d)} \|\Phi\|_{L^2(\mathbb{R}^d)}, \quad s > d, \quad 0 < r < 1.
 \tag{5.35}$$

Since $\mathcal{T}_{b_*}\{f\}(\mathbf{k}) = \langle p_{b_*}(\cdot, \mathbf{k}), \mathcal{T}\{f\}(\cdot, \mathbf{k}) \rangle_{L^2(\Omega)}$, we have by (5.31), (5.32), (5.33), (5.34), and (5.35) that

$$\begin{aligned}
 \mathcal{T}_{b_*}\{Q(\varepsilon \cdot) \Psi_{\text{near}}^\varepsilon(\cdot)\}(\mathbf{k}) &= \frac{1}{\varepsilon^d} \mathcal{F}_{\mathbf{y}} \left\{ Q \chi(|\nabla| \leq \varepsilon^{r-1}) \Phi \right\} \left(\frac{\mathbf{k}}{\varepsilon} \right) + \mathcal{E}(\mathbf{k}), \\
 \|\mathcal{E}\|_{L^2(\mathbb{R}^d)} &\leq C \varepsilon^s \|Q\|_{H^s(\mathbb{R}^d)} \|\Phi\|_{L^2(\mathbb{R}^d)}, \quad s > d, \quad 0 < r < 1,
 \end{aligned}
 \tag{5.36}$$

which is the assertion of Lemma 5.2.

LEMMA 5.3. *The right-hand side of (5.23), defined in (5.24), satisfies*

$$\begin{aligned}
 \widehat{R}_{\text{near}}^\varepsilon[\Psi_{\text{near}}^\varepsilon, \Upsilon^\varepsilon](\mathbf{k}) &= \frac{1}{\varepsilon^d} \chi \left(\left| \frac{\mathbf{k}}{\varepsilon} \right| < \varepsilon^{r-1} \right) \left[\Upsilon^\varepsilon \widehat{F}_{A,Q} \left(\frac{\mathbf{k}}{\varepsilon} \right) + \left\langle w(\cdot), \widehat{U}^\# \left(\cdot, \frac{\mathbf{k}}{\varepsilon} \right) \right\rangle_{L^2(\Omega)} \right] + \mathcal{S}(\mathbf{k}),
 \end{aligned}
 \tag{5.37}$$

where

$$\|\mathcal{S}\|_{L^2(\mathbb{R}^d)} \leq C (\varepsilon + \varepsilon^{2-2r} + \varepsilon^{3r-2}) \|\Phi\|_{L^2(\mathbb{R}^d)}.
 \tag{5.38}$$

Proof. The proof follows in a manner similar to that of Lemma 5.2 by use of (5.3) and (5.26) along with the estimates in Proposition 5.1 and (5.24). \square

5.3. Solution of the near frequency equation for small ε . The results from the previous section enable us to complete the proof of Theorem 3.1.

Substitution of the expansions of Lemmas 5.2 and 5.3 into (5.27) and defining

$$\boldsymbol{\kappa} = \frac{\mathbf{k}}{\varepsilon}
 \tag{5.39}$$

results in the following.

PROPOSITION 5.4. *The near frequency component Φ satisfies the equation*

$$\begin{aligned}
 \mathcal{F}_{\mathbf{y}} \left\{ \left(A_{jl} \partial_{y_j} \partial_{y_l} - e_{A,Q} \right) \chi(|\nabla| < \varepsilon^{r-1}) \Phi \right\}(\boldsymbol{\kappa}) \\
 + \mathcal{F}_{\mathbf{y}} \{ Q \chi(|\nabla| < \varepsilon^{r-1}) \Phi \}(\boldsymbol{\kappa}) &= \mathcal{F}_{\mathbf{y}} H[\Phi, \Upsilon^\varepsilon, \varepsilon].
 \end{aligned}
 \tag{5.40}$$

The right-hand side has the form

$$\begin{aligned}
 FH[\Phi, \Upsilon^\varepsilon, \varepsilon] &= \chi(|\kappa| < \varepsilon^{r-1})(\varepsilon^d \tilde{R}_{near}^\varepsilon[\chi(|\nabla| < \varepsilon^{r-1})\Phi/\varepsilon^d, \Upsilon^\varepsilon] + \tilde{R}_c[\Phi]) \\
 (5.41) \qquad &= \chi(|\kappa| < \varepsilon^{r-1}) \left[\Upsilon^\varepsilon \widehat{F}_{A,Q}(\kappa) + \left\langle w(\cdot), \widehat{U}^\#(\cdot, \kappa) \right\rangle_{L^2(\Omega)} \right. \\
 &\qquad \qquad \qquad \left. + \mathcal{O}(\varepsilon^r + \varepsilon^{2-2r} + \varepsilon^{3r-2}) \right].
 \end{aligned}$$

We define the operators $\chi_\varepsilon, \bar{\chi}_\varepsilon$:

$$(5.42) \qquad \chi_\varepsilon \equiv \chi(|\nabla_{\mathbf{y}}| < \varepsilon^{r-1}), \quad \bar{\chi}_\varepsilon \equiv 1 - \chi_\varepsilon = \chi(|\nabla_{\mathbf{y}}| \geq \varepsilon^{r-1}).$$

In physical space we can write (5.40) as

$$(5.43) \qquad \chi_\varepsilon L_{A,Q} \chi_\varepsilon \Phi = \chi_\varepsilon H[\Phi, \Upsilon^\varepsilon, \varepsilon],$$

where

$$\begin{aligned}
 (5.44) \qquad H[\Phi, \Upsilon^\varepsilon, \varepsilon](\mathbf{y}) &= \Upsilon^\varepsilon F_{A,Q}(\mathbf{y}) + \left\langle w(\cdot), U^\#(\cdot, \mathbf{y}) \right\rangle_{L^2(\Omega)} + h[\Phi, \Upsilon^\varepsilon, \varepsilon], \\
 \|\chi_\varepsilon h[\Phi, \Upsilon^\varepsilon, \varepsilon]\|_{H^2(\mathbb{R}^d)} &\leq C(\varepsilon^r + \varepsilon^{2-2r} + \varepsilon^{3r-2})(1 + \|\Phi\|_{H^2(\mathbb{R}^d)}).
 \end{aligned}$$

In order to solve (5.43), we require a regularization that guarantees the invertibility of the operator $\chi_\varepsilon L_{A,Q} \chi_\varepsilon$. Since zero is an isolated eigenvalue of $L_{A,Q}$, there is a small disc of radius $\rho = \rho_\varepsilon$ about zero, with boundary C_ρ such that for ε sufficiently small, C_ρ encircles m eigenvalues of $\chi_\varepsilon L_{A,Q} \chi_\varepsilon$, counting multiplicity, where m is the multiplicity of zero as an eigenvalue of $L_{A,Q}$.

Introduce the projection onto the spectral subspace associated with eigenvalues of $\chi_\varepsilon L_{A,Q} \chi_\varepsilon$, encircled by C_ρ :

$$(5.45) \qquad \Pi_\varepsilon \equiv \frac{1}{2\pi i} \int_{C_\rho} (\chi_\varepsilon L_{A,Q} \chi_\varepsilon - \lambda I)^{-1} d\lambda.$$

Note that

$$(5.46) \qquad \Pi_0 = \langle F_{A,Q}, \cdot \rangle_{L^2(\mathbb{R}^d)}$$

projects onto the kernel of $L_{A,Q}$.

We now rewrite (5.43) as the following system for Φ and Υ^ε :

$$(5.47) \qquad \chi_\varepsilon L_{A,Q} \chi_\varepsilon \Phi = \chi_\varepsilon (I - \Pi_\varepsilon) \chi_\varepsilon H[\Phi, \Upsilon^\varepsilon, \varepsilon],$$

$$(5.48) \qquad \chi_\varepsilon \Pi_\varepsilon \chi_\varepsilon H[\Phi, \Upsilon^\varepsilon, \varepsilon] = 0.$$

Any solution $(\Phi^\varepsilon, \Upsilon^\varepsilon)$ of (5.47), (5.48) is a solution of (5.43).

We claim that for ε small (5.47) can be solved for $\Phi = \Phi^\varepsilon[\Upsilon^\varepsilon]$ via the equivalent nonlocal “integral” equation:

$$(5.49) \qquad \Phi^\varepsilon = (\chi_\varepsilon L_{A,Q} \chi_\varepsilon)^{-1} (I - \Pi_\varepsilon) \left(\Upsilon^\varepsilon F_{A,Q} + \left\langle w(\cdot), U^\#(\cdot, \mathbf{y}) \right\rangle_{L^2(\mathbb{R}^d)} + h[\Phi^\varepsilon, \Upsilon^\varepsilon, \varepsilon] \right).$$

Indeed, the solution may be constructed using the iteration

$$\begin{aligned}
 (5.50) \qquad \Phi_{j+1}^\varepsilon &= (\chi_\varepsilon L_{A,Q} \chi_\varepsilon)^{-1} \chi_\varepsilon (I - \Pi_\varepsilon) \chi_\varepsilon \left(\Upsilon^\varepsilon F_{A,Q} + \left\langle w(\cdot), U^\#(\cdot, \mathbf{y}) \right\rangle_{L^2(\mathbb{R}^d)} + h[\Phi_j^\varepsilon, \Upsilon^\varepsilon, \varepsilon] \right), \\
 \Phi_0^\varepsilon &= (\chi_\varepsilon L_{A,Q} \chi_\varepsilon)^{-1} \chi_\varepsilon (I - \Pi_\varepsilon) \left(\Upsilon^\varepsilon F_{A,Q} + \left\langle w(\cdot), U^\#(\cdot, \mathbf{y}) \right\rangle_{L^2(\mathbb{R}^d)} \right).
 \end{aligned}$$

By use of (5.45) and (5.44), we have

$$\begin{aligned} \|\Phi_{j+1} - \Phi_j\| &\leq \|(\chi_\varepsilon L_{A,Q} \chi_\varepsilon)^{-1} \chi_\varepsilon (I - \Pi_\varepsilon) \chi_\varepsilon (h[\Phi_j, \Upsilon^\varepsilon, \varepsilon] - h[\Phi_{j-1}, \Upsilon^\varepsilon, \varepsilon])\| \\ &\leq \tau(\varepsilon) \|\Phi_j - \Phi_{j-1}\|, \quad \tau(\varepsilon) \equiv \rho^{-1} C(\varepsilon^r + \varepsilon^{2-2r} + \varepsilon^{3r-2}), \quad \frac{2}{3} < r < 1. \end{aligned}$$

Therefore, $\|\Phi_{j+1} - \Phi_j\| \leq \tau(\varepsilon)^j \|\Phi_1 - \Phi_0\|$, and if ε satisfies the smallness condition $\tau(\varepsilon) < 1$, the sequence $\{\Phi_j^\varepsilon\}_{j \geq 0}$ is Cauchy in $H^2(\mathbb{R}^d)$. It therefore contains a subsequence, which is convergent to a limit $\Phi_*^\varepsilon \in H^2(\mathbb{R}^d)$. By $H^2(\mathbb{R}^d)$ continuity of the terms in the iteration (5.50), one can pass to the limit in (5.50) to obtain a solution Φ_*^ε which satisfies (5.49).

This solution Φ_*^ε is a functional of Υ^ε and appears in (5.48), which we view as an equation for Υ^ε . We write (5.48) in the form

$$\begin{aligned} (5.51) \quad g[v, \varepsilon] &\equiv v \chi_\varepsilon \Pi_\varepsilon F_{A,Q}(\mathbf{y}) + \chi_\varepsilon \Pi_\varepsilon \langle w(\cdot), U^\#(\cdot, \mathbf{y}) \rangle_{L^2(\Omega)} \\ &\quad + \chi_\varepsilon \Pi_\varepsilon h[\Phi[v], v, \varepsilon] = 0. \end{aligned}$$

For $\varepsilon = 0$, this equation has the solution $g[v_0, 0] = 0$ with

$$(5.52) \quad v_0 = - \left\langle F_{A,Q}(\cdot), \langle w(\circ), U^\#(\circ, \cdot) \rangle_{L^2(\Omega)} \right\rangle_{L^2(\mathbb{R}^d)}.$$

The Jacobian is $D_v g[v_0, 0] = 1$. By the implicit function theorem [23], for $|\varepsilon|$ sufficiently small there exists a unique solution $\varepsilon \mapsto \Upsilon^\varepsilon$ satisfying $g[\Upsilon^\varepsilon, \varepsilon] = 0$. This completes the proof of Theorem 3.1.

Appendix A. Effective mass tensor. In this appendix we prove Proposition 4.4, relating the Hessian matrix of the band dispersion function $E_{b_*}(\mathbf{k})$ to the matrix A resulting from the multiple-scale analysis. In addition, we prove hypothesis H2(b) under certain conditions and the positive definiteness of $I - A$.

The solutions to the eigenvalue equation (2.5) are sought in the form $u_b(\mathbf{x}; \mathbf{k}) = e^{2\pi i \mathbf{k} \cdot \mathbf{x}} p_b(\mathbf{x}; \mathbf{k})$, $\mathbf{k} \in \Omega_*$. Then p_{b_*} and E_{b_*} satisfy

$$(A.1) \quad L_*^{(\mathbf{k})} p_{b_*} \equiv (-\Delta - 4\pi i \mathbf{k} \cdot \nabla + 4\pi^2 |\mathbf{k}|^2 + V(\mathbf{x}) - E_{b_*}(\mathbf{k})) p_{b_*}(\mathbf{x}, \mathbf{k}) = 0, \quad \mathbf{x} \in \mathbb{T}^d,$$

with periodic boundary conditions $p_{b_*}(\mathbf{x} + \mathbf{e}_j; \mathbf{k}) = p_{b_*}(\mathbf{x}; \mathbf{k})$. Taking the derivative of (A.1) with respect to k_j gives

$$(A.2) \quad L_*^{(\mathbf{k})} \partial_{k_j} p_{b_*}(\mathbf{x}; \mathbf{k}) = (4\pi i \partial_{x_j} - 8\pi^2 k_j + \partial_{k_j} E_{b_*}(\mathbf{k})) p_{b_*}(\mathbf{x}; \mathbf{k}).$$

Evaluating (A.2) at $\mathbf{k} = \mathbf{k}_*$ and using the fact that the kernel of $L_*^{(\mathbf{k}_*)}$ is spanned by $p_{b_*}(\mathbf{x}; \mathbf{k}_*)$, we arrive at the solvability condition

$$(A.3) \quad \partial_{k_j} E_{b_*}(\mathbf{k}_*) = -4\pi i \langle (\partial_{x_j} + 2\pi i k_{*,j}) p_{b_*}(\cdot; \mathbf{k}_*), p_{b_*}(\cdot; \mathbf{k}_*) \rangle_{L^2(\Omega)}$$

for $j = 1, 2, \dots, d$. When $\mathbf{k}_* = 0$, $p_{b_*}(\mathbf{x}; \mathbf{k}_*)$ is real valued so that (A.3) simplifies to

$$(A.4) \quad \partial_{k_j} E_{b_*}(\mathbf{k}_*) = 0, \quad j = 1, 2, \dots, d.$$

For the case $d = 1$, we also have

$$(A.5) \quad E'_{b_*}(k_*) = 0, \quad k_* \in \{0, \pm 1/2\}, \quad d = 1.$$

This result follows from properties of the Floquet discriminant $\Delta(E)$ [12]. Briefly, for each E , one constructs a 2×2 fundamental matrix of solutions $M(E)$ and considers the values of E for which $M(E)$ has an eigenvalue 1 or -1 corresponding to a periodic or antiperiodic eigenvalue, respectively. This is equivalent to $\Delta(E) = \pm 2$, where

$$(A.6) \quad \text{trace}(M(E_b(k))) = \Delta(E_b(k)) = 2 \cos(2\pi k(E_b)).$$

Differentiating this expression with respect to k and evaluating at $k = k_*$ gives

$$(A.7) \quad \frac{d\Delta}{dE}(E_{b_*}(k)) E'_{b_*}(k) = -4\pi \sin(2\pi k).$$

Since $d\Delta/dE(E) = 0$ if and only if E is a double eigenvalue [12, Theorem 2.3.1] and $E_{b_*}(k_*)$ is assumed simple (hypothesis H2(a)), (A.5) follows.

The above discussion proves hypothesis H2(b) at the left band edge $\mathbf{k}_* = 0$ for arbitrary d and both left and right band edges $k_* \in \{0, \pm 1/2\}$ when $d = 1$. It is possible for $\nabla E_{b_*}(\mathbf{k}_*) = 0$ in other cases, e.g., separable potentials, and we continue the discussion assuming this to be true.

It follows that

$$(A.8) \quad \partial_{k_j} p_{b_*}(\mathbf{x}; \mathbf{k}_*) = 4\pi i (L_*^{(\mathbf{k}_*)})^{-1} \{(\partial_{x_j} + 2\pi i k_{*,j}) p_{b_*}(\cdot; \mathbf{k}_*)\}(\mathbf{x}).$$

Differentiating (A.2) with respect to k_l and setting $\mathbf{k} = \mathbf{k}_*$ gives

$$(A.9) \quad \begin{aligned} L_*^{(\mathbf{k}_*)} \partial_{k_j} \partial_{k_l} p_{b_*}(\mathbf{x}; \mathbf{k}_*) \\ = -16\pi^2 (\partial_{x_l} + 2\pi i k_{*,l}) (L_*^{(\mathbf{k}_*)})^{-1} \{(\partial_{x_j} + 2\pi i k_{*,j}) p_{b_*}(\cdot; \mathbf{k}_*)\}(\mathbf{x}) \\ - 16\pi^2 (\partial_{x_j} + 2\pi i k_{*,j}) (L_*^{(\mathbf{k}_*)})^{-1} \{(\partial_{x_l} + 2\pi i k_{*,l}) p_{b_*}(\cdot; \mathbf{k}_*)\}(\mathbf{x}) \\ + (\partial_{k_j k_l} E_{b_*}(\mathbf{k}_*) - 8\pi^2 \delta_{jl}) p_{b_*}(\mathbf{x}; \mathbf{k}_*). \end{aligned}$$

Invoking the solvability condition and using $\|p_{b_*}\|_{L^2(\Omega)} = 1$, (A.4) gives

$$(A.10) \quad \begin{aligned} \partial_{k_j k_l} E_{b_*}(\mathbf{k}_*) &= 8\pi^2 \delta_{jl} \\ &+ 16\pi^2 \left\langle (\partial_{x_l} + 2\pi i k_{*,l}) (L_*^{(\mathbf{k}_*)})^{-1} \{(\partial_{x_j} + 2\pi i k_{*,j}) p_{b_*}(\cdot; \mathbf{k}_*)\}(\cdot), p_{b_*}(\cdot; \mathbf{k}_*) \right\rangle_{L^2(\Omega)} \\ &+ 16\pi^2 \left\langle (\partial_{x_j} + 2\pi i k_{*,j}) (L_*^{(\mathbf{k}_*)})^{-1} \{(\partial_{x_l} + 2\pi i k_{*,l}) p_{b_*}(\cdot; \mathbf{k}_*)\}(\cdot), p_{b_*}(\cdot; \mathbf{k}_*) \right\rangle_{L^2(\Omega)}. \end{aligned}$$

Integrating by parts and using the fact that $(L_*^{(\mathbf{k}_*)})^{-1}$ is self-adjoint, the last two terms are equal, giving

$$(A.11) \quad \begin{aligned} \partial_{k_j k_l} E_{b_*}(\mathbf{k}_*) &= 8\pi^2 \delta_{jl} \\ &- 32\pi^2 \left\langle (\partial_{x_j} + 2\pi i k_{*,j}) p_{b_*}(\cdot; \mathbf{k}_*), (L_*^{(\mathbf{k}_*)})^{-1} \{(\partial_{x_l} + 2\pi i k_{*,l}) p_{b_*}(\cdot; \mathbf{k}_*)\}(\cdot) \right\rangle_{L^2(\Omega)}. \end{aligned}$$

In order to identify (A.11) with the final result, (4.20) in Proposition 4.4, we use the definition of $w(\mathbf{x})$ in (2.9) to compute

$$(A.12) \quad \partial_{x_j} w(\mathbf{x}) = e^{2\pi i \mathbf{k}_* \cdot \mathbf{x}} (\partial_{x_j} + 2\pi i k_{*,j}) p_{b_*}(\mathbf{x}; \mathbf{k}_*),$$

which is the first term in the inner product of (A.12). In addition, the identity

$$(A.13) \quad L_* e^{2\pi i \mathbf{k}_* \cdot \mathbf{x}} f(\mathbf{x}) = e^{2\pi i \mathbf{k}_* \cdot \mathbf{x}} L_*^{(\mathbf{k}_*)} f(\mathbf{x})$$

implies

$$(A.14) \quad e^{2\pi i \mathbf{k}_* \cdot \mathbf{x}} (L_*^{(\mathbf{k}_*)})^{-1} \{(\partial_{x_l} + 2\pi i k_{*,l}) p_{b_*}(\cdot; \mathbf{k}_*)\}(\mathbf{x}) = L_*^{-1} \{\partial_{x_l} w(\cdot)\}(\mathbf{x}),$$

and the result follows.

Appendix B. Homogenization and variational analysis. The existence of a bound state for (1.1) bifurcating from the lowest band edge $E_0(0)$ can be proved by showing that the Rayleigh quotient

$$(B.1) \quad \mathcal{E}[u] = \frac{\int_{\mathbb{R}^d} \{|\nabla u(\mathbf{x})|^2 + [V(\mathbf{x}) + \varepsilon^2 Q(\varepsilon \mathbf{x}) - E_0(0)]|u(\mathbf{x})|^2 d\mathbf{x}\}}{\int_{\mathbb{R}^d} |u(\mathbf{x})|^2 d\mathbf{x}}$$

is negative for some choice of $u \in H^1(\mathbb{R}^d)$ [21]. A natural choice for u is the multiscale expansion in (4.2) with ε sufficiently small. Furthermore, a higher order, two-term trial function gives a better approximation of the energy than the one-term trial function.

PROPOSITION B.1.

1. Negative energy trial function: *With assumptions H1–H3 in section 3 and setting $E_* \equiv E_0(0)$, the lowest band edge, then there exists $\varepsilon_0 > 0$ such that for all $0 < \varepsilon < \varepsilon_0$,*

$$(B.2) \quad \mathcal{E} [F_{A,Q}(\varepsilon \circ) w(\circ) + 2\nabla_{\circ} F_{A,Q}(\varepsilon \circ) \cdot L_*^{-1} \{\nabla w\}(\circ)] < 0.$$

It follows that there exists a ground state.

2. Estimates of the ground state energy: *If $L_{I,Q} \equiv -\Delta_{\mathbf{y}} + Q(\mathbf{y})$ has a simple eigenvalue $e_{I,Q} < 0$ and corresponding eigenfunction $F_{I,Q}(\mathbf{y}) \in H^2(\mathbb{R}^d)$, then there exists $\varepsilon_0 > 0$ such that for all $0 < \varepsilon < \varepsilon_0$,*

$$(B.3) \quad \mathcal{E} [F_{A,Q}(\varepsilon \circ) w(\circ) + 2\nabla_{\circ} F_{A,Q}(\varepsilon \circ) \cdot L_*^{-1} \{\nabla w\}(\circ)] < \mathcal{E} [F_{I,Q}(\varepsilon \circ) w(\circ)] < 0.$$

Proof. For the proof of Proposition B.1, we will make repeated use of the following averaging lemma.

LEMMA B.2. *Let $p(\mathbf{x}) = p(\mathbf{x} + \mathbf{z})$ be periodic with fundamental period cell Ω and $\sum_{\mathbf{z} \in \mathbb{Z}^d} |\hat{p}_{\mathbf{z}}| < \infty$, where $\hat{p}_{\mathbf{z}}$ are the Fourier series coefficients of $p(\mathbf{x})$. If $G \in L^1(\mathbb{R}^d) \cap C^n(\mathbb{R}^d)$, then*

$$(B.4) \quad \left| \int_{\mathbb{R}^d} p(\mathbf{x}) G(\varepsilon \mathbf{x}) d\mathbf{x} - \frac{1}{\varepsilon^d} \int_{\Omega} p(\mathbf{x}) d\mathbf{x} \int_{\mathbb{R}^d} G(\mathbf{y}) d\mathbf{y} \right| \leq C\varepsilon^n.$$

Proof. Expand p in the Fourier series $p(\mathbf{x}) = \sum_{\mathbf{z} \in \mathbb{Z}^d} \hat{p}_{\mathbf{z}} e^{2\pi i \mathbf{z} \cdot \mathbf{x}}$. Then

$$(B.5) \quad \begin{aligned} \int_{\mathbb{R}^d} p(\mathbf{x}) G(\varepsilon \mathbf{x}) d\mathbf{x} &= \frac{1}{\varepsilon^d} \sum_{\mathbf{z} \in \mathbb{Z}^d} \hat{p}_{\mathbf{z}} \int_{\mathbb{R}^d} G(\mathbf{y}) e^{2\pi i \mathbf{z} \cdot \mathbf{y} / \varepsilon} d\mathbf{y} \\ &= \frac{\hat{p}_0}{\varepsilon^d} \int_{\mathbb{R}^d} G(\mathbf{y}) d\mathbf{y} + \frac{1}{\varepsilon^d} \sum_{\mathbf{z} \neq 0} \hat{p}_{\mathbf{z}} \int_{\mathbb{R}^d} G(\mathbf{y}) e^{2\pi i \mathbf{z} \cdot \mathbf{y} / \varepsilon} d\mathbf{y} \\ &= \frac{1}{\varepsilon^d} \int_{\Omega} p(\mathbf{x}) d\mathbf{x} \int_{\mathbb{R}^d} G(\mathbf{y}) d\mathbf{y} + \mathcal{O}(\varepsilon^n), \end{aligned}$$

where the first line is justified by the assumed absolute convergence of the Fourier coefficients and the second line results from integration by parts n times. \square

First we consider the ansatz $u(\mathbf{x}) = F_{I,Q}(\varepsilon\mathbf{x})w(\mathbf{x})$ for (B.3). A computation and several applications of the averaging lemma, Lemma B.2, give

$$(B.6) \quad \begin{aligned} \mathcal{E} [F_{I,Q}(\varepsilon\circ)w(\circ)] &= \varepsilon^2 \frac{\int_{\mathbb{R}^d} \{ |\nabla F_{I,Q}(\mathbf{y})|^2 + Q(\mathbf{y})|F_{I,Q}(\mathbf{y})|^2 \} d\mathbf{y}}{\int_{\mathbb{R}^d} |F_{I,Q}(\mathbf{y})|^2 d\mathbf{y}} + o(\varepsilon^2) \\ &= \varepsilon^2 e_{I,Q} + o(\varepsilon^2) < 0 \end{aligned}$$

for ε sufficiently small.

A similar, more involved computation for the ansatz $u(\mathbf{x}) = F_{A,Q}(\varepsilon\mathbf{x})w(\mathbf{x}) + 2\nabla F_{A,Q}(\varepsilon\mathbf{x}) \cdot L_*^{-1} \{ \nabla w \}(\mathbf{x})$ leads to

$$(B.7) \quad \begin{aligned} &\mathcal{E} [F_{A,Q}(\varepsilon\circ)w(\circ) + 2\nabla F_{A,Q}(\varepsilon\circ) \cdot L_*^{-1} \{ \nabla w \}(\circ)] \\ &= \varepsilon^2 \frac{\int_{\mathbb{R}^d} \{ \nabla F_{A,Q}(\mathbf{y}) \cdot A \nabla F_{A,Q}(\mathbf{y}) + Q(\mathbf{y})|F_{A,Q}(\mathbf{y})|^2 \} d\mathbf{y}}{\int_{\mathbb{R}^d} |F_{A,Q}(\mathbf{y})|^2 d\mathbf{y}} + o(\varepsilon^2) \\ &= \varepsilon^2 e_{A,Q} + o(\varepsilon^2) < 0 \end{aligned}$$

for ε sufficiently small. For a bifurcation from the lowest band edge, the effective mass tensor A is positive definite [19], and hence the eigenvalue $e_{A,Q}$ is negative.

The proof of Proposition B.1 is complete if we can show that $e_{A,Q} < e_{I,Q}$. For this, we use the following proposition.

PROPOSITION B.3. *The operator $I - A = (4 \langle \partial_{x_j} w, L_*^{-1} \{ \partial_{x_i} w \} \rangle_{L^2(\Omega)})$ is positive definite at the lowest band edge ($b_* = 0, \mathbf{k}_* = 0$).*

Proof. Recall that $L_* \geq 0$ with one-dimensional $L^2(\mathbb{T}^d)$ kernel spanned by w . Let $\mathbf{v} = (v_1, \dots, v_d) \in \mathbb{R}^d$ be arbitrary. Then

$$(B.8) \quad \mathbf{v} \cdot (I - A)\mathbf{v} = \langle \mathbf{v} \cdot \nabla w, L_*^{-1} \mathbf{v} \cdot \nabla w \rangle_{L^2(\Omega)} \geq \frac{1}{E_1(0) - E_*} \|\mathbf{v} \cdot \nabla w\|^2 \geq C \|\mathbf{v}\|^2, \quad C > 0,$$

where $E_1(0) - E_* > 0$ is the second eigenvalue of L_* acting on $L^2(\mathbb{T}^d)$. \square

Introducing the energy functional

$$(B.9) \quad J_{A,Q}[g] \equiv \frac{\int_{\mathbb{R}^d} [\nabla g(\mathbf{y}) \cdot A \nabla g(\mathbf{y}) + Q(\mathbf{y})g^2(\mathbf{y})] d\mathbf{y}}{\int_{\mathbb{R}^d} g^2(\mathbf{y}) d\mathbf{y}}, \quad g \in L^2(\Omega),$$

we observe

$$(B.10) \quad J_{A,Q}[g] - J_{I,Q}[g] = \frac{\int_{\mathbb{R}^d} [\nabla g(\mathbf{y}) \cdot (A - I) \nabla g(\mathbf{y})] d\mathbf{y}}{\int_{\mathbb{R}^d} g^2(\mathbf{y}) d\mathbf{y}} < 0, \quad g \in L^2(\Omega),$$

by the negative definiteness of $A - I$ from Proposition B.3. Using (B.6), (B.7), and (B.10) we find

$$(B.11) \quad e_{A,Q} = J_{A,Q}[F_{A,Q}] = \inf_{g \in L^2(\Omega)} J_{A,Q}[g] \leq J_{A,Q}[F_{I,Q}] < J_{I,Q}[F_{I,Q}] = e_{I,Q},$$

and the proof is complete. \square

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