

DEFECT MODES AND HOMOGENIZATION OF PERIODIC SCHRODINGER OPERATORS

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Abstract. We consider the discrete eigenvalues of the operator $H_\varepsilon = -\Delta + V(\mathbf{x}) + \varepsilon^2 W(\varepsilon\mathbf{x})$, where $V(\mathbf{x})$ is periodic and $W(\mathbf{y})$ is localized on \mathbb{R}^d .

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

$$H$$



Our results concern a particular class of weak defects, slowly varying and of small amplitude: ${}^2Q(\epsilon)$, 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, ${}^2Q(\epsilon)$, 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. We note that we may, without loss of generality, restrict ourselves to the case where the fundamental period cell is $\mathcal{B} = [0, 1]^d$. Indeed, let \mathcal{B} denote the fundamental period cell, spanned by the linearly independent vectors $\{z_1, \dots, z_d\}$ and define the constant matrix \mathcal{R}^{-1} to be the matrix whose j th column is z_j . Then, under the change of coordinates $x \mapsto z = \mathcal{R}^{-1}x$,

$$\begin{aligned} & \Delta_x \cdot \Delta_x + V(x) \text{ acting on } L^2(\mathcal{B}) \text{ transforms to} \\ & \Delta_z \cdot \Delta_z + \tilde{V}(z) \equiv \sum_{j=1}^d \frac{\partial^2}{\partial z_j^2} + \tilde{V}(z) \\ & \text{acting on } L^2([0, 1]^d), \text{ where} \\ & \tilde{V}(z) = V(\mathcal{R}^{-1}z), \quad \Delta_z = \mathcal{R}^{-1} \Delta_x. \end{aligned}$$

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

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

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

3. $\mathcal{B} = [0, 1]^d$ is the fundamental period cell; $\mathcal{B}^* = [-1/2, 1/2]^d$ is the dual fundamental cell or Brillouin zone.
4. $1 \leq d \leq 3$

6. Fourier spectral cuto :

We will study the bifurcation of eigenvalues from the band edge

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

with the associated, real-valued band edge eigenfunction

$$(2.9) \quad w(\mathbf{x}) \equiv e^{2\pi i \mathbf{k} \cdot \mathbf{x}} \rho_*(\mathbf{x}; \mathbf{k}) \in L^2(\mathbb{T}^d).$$

For example, the lowest band edge is $E_0(0)$ and the associated eigenfunction is periodic $\rho_0(\mathbf{x})$.

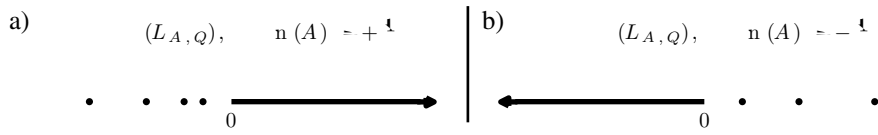


Fig. 3.1. Discrete and continuous spectrum of $L_{A,Q}$. (a) Positive definite effective mass tensor. (b) Negative definite effective mass tensor.

Set $\text{sgn}(A) = +1$ if A is positive definite and $\text{sgn}(A) = -1$ if A is negative definite. Assume L has a simple eigenvalue e with $\text{sgn}(A)e < 0$ and corresponding eigenfunction

Remark 3.4 (branches emanating from degenerate eigenvalues of L_ϵ). In spatial dimensions, $d > 1$, the operator L_ϵ may have degenerate eigenvalues, e.g., if there is symmetry in $Q(\cdot)$. Suppose e_ϵ has multiplicity M . Then, since L_ϵ is self-adjoint, e_ϵ perturbs, generically, to M distinct branches. Thus, applying the method of proof of Theorem 3.1, each degenerate eigenvalue of L_ϵ 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 $\mathcal{O}(\epsilon^3)$ about $E + \epsilon^2 e_\epsilon$. The j th eigenbranch satisfies the error estimates

$$(3.5) \quad \begin{aligned} \|u^{(j)}(\cdot; \mu^{(j)}) - U^{(j)}(\cdot, \cdot)\|_{L^2(\mathbb{R}^d)} &\leq \epsilon^{-1} C, \\ \mu^{(j)} - E - \epsilon^2 e_\epsilon &\leq \epsilon^3 C \end{aligned}$$

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 OF A GAP. 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 $u(\cdot; \mu)$ satisfies (1.1),

$$(4.1) \quad [-\Delta + V(\cdot) + \epsilon^2 Q(\cdot)]u = \mu u,$$

and expand it in an asymptotic series as follows:

$$(4.2) \quad u(\cdot; \mu) = U_\epsilon(\cdot, \cdot) = \sum_0 U(\cdot, \cdot), \quad \mu = E + \sum_1 \mu,$$

where $\cdot = \cdot$ is the slow variable. Treating \cdot and \cdot as independent variables, (4.1) then takes the form

(4.3)

Viewed as a system of partial differential equations for functions of the fast variable

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

$$(4.16) \quad L U_2 = 2 \cdot_j F_1 \cdot_j W \quad \mathcal{L}[F_0],$$

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

$$(4.17) \quad \mathcal{L}[G](\cdot, \cdot) = 4 \cdot_j L^{-1}\{\cdot_i W\}(\cdot) \cdot_j \cdot_i G(\cdot) + w(\cdot)[-\Delta_y + Q(\cdot) - \mu_2]G(\cdot).$$

Definition 4.3. Define the operator $L : H^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ by

$$(4.18) \quad L G(\cdot) \equiv \langle w(\cdot), \mathcal{L}[G](\cdot, \cdot) \rangle_{L^2(\Omega)} = [-\Delta_y \cdot A - \Delta_y + Q(\cdot) - e]G(\cdot),$$

where e is the simple eigenvalue associated with the eigenfunction $F(\cdot)$ in hypothesis H3 and

$$(4.19) \quad A \equiv 4 \cdot_j W, L^{-1}\{\cdot_i W\} \rangle_{L^2(\Omega)}.$$

Proposition 4.4.

$$(4.20) \quad A = \frac{1}{8} 2 \cdot_j \cdot_i E_*(\cdot).$$

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

Applying Proposition 4.1 to (4.16) gives

$$(4.21) \quad \langle w(\cdot), \mathcal{L}[F_0](\cdot, \cdot) \rangle_{L^2(\Omega)} = 0 \Leftrightarrow L F_0 = 0, \quad \mu_2 = e,$$

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 $F \in H^2(\mathbb{R}^d)$ and $e \in \mathbb{R} \setminus \{0\}$. Thus, $F_0(\cdot) = F(\cdot)$.

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

$$(4.22) \quad U_2(\cdot, \cdot) = w(\cdot)F_2(\cdot) + 2 \cdot_j F_1(\cdot) L^{-1}\{\cdot_i W\}(\cdot) + L^{-1}\{\mathcal{L}[F_0](\cdot, \cdot)\}(\cdot).$$

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

$$(4.23) \quad L U_3 = 2 \cdot_j F_2 \cdot_j W \quad \mathcal{L}[F_1] \quad \mathcal{H}_3 + \mu_3 W F,$$

where \mathcal{H}_3 is known:

$$(4.24) \quad \mathcal{H}_3(\cdot, \cdot) = 2 \cdot_j \cdot_j L^{-1}\{\mathcal{L}[F_0](\cdot, \cdot)\}(\cdot) + 2L^{-1}\{\cdot_i W\}(\cdot)[-\Delta_y + Q(\cdot) - e] \cdot_j F(\cdot).$$

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

$$(4.25) \quad L F_1 = \langle w(\cdot), \mathcal{H}_3(\cdot, \cdot) \rangle_{L^2(\Omega)} + \mu_3 F.$$

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

$$(4.26) \quad \mu_3 = F(\cdot), \langle w(\cdot), \mathcal{H}_3(\cdot, \cdot) \rangle_{L^2(\Omega)} \rangle_{L^2(\mathbb{R}^d)}.$$

We can now write F_1 in terms of F as

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

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

$$(4.28) \quad U_3(\cdot, \cdot) = w(\cdot) F_3(\cdot) + 2 \cdot_j F_2(\cdot) L^{-1} \{ \cdot_j w \}(\cdot) \\ L^{-1} \left(\mathcal{L}[F_1](\cdot, \cdot) + \mathcal{H}_3(\cdot, \cdot) - \mu_3 w(\cdot) F(\cdot) \right),$$

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

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

$$(4.29) \quad L U = 2 \cdot_j F_{-1} \cdot_j w \mathcal{L}[F_{-2}] \mathcal{H} + \mu w F,$$

where \mathcal{H}

edge and “far” from the band edge:

$$\begin{aligned}
 (5.5) \quad & \tilde{u}(\mathbf{k}; \omega) = \tilde{u}(\mathbf{k}; \omega) + \tilde{u}(\mathbf{k}; \omega) = \mathcal{T}^{-1} \tilde{u}(\mathbf{k}; \omega) + \mathcal{T}^{-1} \tilde{u}(\mathbf{k}; \omega), \\
 & \tilde{u}(\mathbf{k}; \omega) = \tilde{u}(\mathbf{k}; \omega) \equiv \left(\mathbf{k} \cdot \mathbf{k}_* < \omega \right) \mathcal{T}_* \{ \tilde{u}(\mathbf{k}; \omega) \} p_*(\mathbf{k}; \omega), \\
 & \tilde{u}(\mathbf{k}; \omega) = \tilde{u}(\mathbf{k}; \omega) \equiv \left(\mathbf{k} \cdot \mathbf{k}_* \geq \omega \right) \mathcal{T} \{ \tilde{u}(\mathbf{k}; \omega) \} p(\mathbf{k}; \omega),
 \end{aligned}$$

where $\delta_{\mathbf{k}, \mathbf{k}_*}$ is the Kronecker delta function and the indicator functions are defined as

$$(5.6) \quad \left(\mathbf{k} \cdot \mathbf{k}_* < \omega \right) \equiv 1_{\{\mathbf{k} \cdot \mathbf{k}_* < \omega\}}(\mathbf{k}), \quad \left(\mathbf{k} \cdot \mathbf{k}_* \geq \omega \right) \equiv 1_{\{\mathbf{k} \cdot \mathbf{k}_* \geq \omega\}}(\mathbf{k}).$$

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

We will use the conventions

$$\begin{aligned}
 (5.7) \quad & \tilde{u}(\mathbf{k}; \omega) \equiv p_*(\mathbf{k}; \omega), \quad \tilde{u}(\mathbf{k}; \omega) \equiv \tilde{u}(\mathbf{k}; \omega)_{2(\Omega)}, \\
 & \tilde{u}(\mathbf{k}; \omega) \equiv p(\mathbf{k}; \omega), \quad \tilde{u}(\mathbf{k}; \omega) \equiv \tilde{u}(\mathbf{k}; \omega)_0,
 \end{aligned}$$

where $\tilde{u}(\mathbf{k}; \omega)$ is a scalar and $\tilde{u}(\mathbf{k}; \omega)$ is an infinite vector. This decomposition was used in [10, 9, 16]. The parameter r is assumed to lie in the interval

$$(5.8) \quad r \in (2/3, 1),$$

the choice of which will be made clear later.

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

$$\begin{aligned}
 (5.9) \quad & [E(\mathbf{k}; \omega) - E_*(\mathbf{k}; \omega) - 2e^{-i\mathbf{k} \cdot \mathbf{k}_*}] \mathcal{T} \{ \tilde{u}(\mathbf{k}; \omega) \} + 2 \mathcal{T} \{ Q(\cdot; \omega) \tilde{u}(\mathbf{k}; \omega) \}(\mathbf{k}) \\
 & = 2 \mathcal{T} \{ R[\mathbf{k}; \omega] \}(\mathbf{k}), \quad b = 0, 1, \dots
 \end{aligned}$$

We view this as a coupled system of equations for the near and far frequency components $\tilde{u}(\mathbf{k}; \omega)$ and $\tilde{u}(\mathbf{k}; \omega)$, $\omega \in \mathbb{R}$:

$$\begin{aligned}
 (5.10) \quad \text{near:} \quad & (E_*(\mathbf{k}; \omega) - E_*(\mathbf{k}; \omega) - 2e^{-i\mathbf{k} \cdot \mathbf{k}_*}) \tilde{u}(\mathbf{k}; \omega) \\
 & + 2 \left(\mathbf{k} \cdot \mathbf{k}_* < \omega \right) \mathcal{T}_* \{ Q(\cdot; \omega) \tilde{u}(\mathbf{k}; \omega) \}(\mathbf{k}) \\
 & = 2 \left(\mathbf{k} \cdot \mathbf{k}_* < \omega \right) \mathcal{T}_* \{ Q(\cdot; \omega) \tilde{u}(\mathbf{k}; \omega) \}(\mathbf{k}) \\
 & + \mathcal{T}_* \{ R[\mathbf{k}; \omega] \}(\mathbf{k}),
 \end{aligned}$$

$$\begin{aligned}
 (5.11) \quad \text{far:} \quad & (E(\mathbf{k}; \omega) - E_*(\mathbf{k}; \omega) - 2e^{-i\mathbf{k} \cdot \mathbf{k}_*}) \tilde{u}(\mathbf{k}; \omega) \\
 & + 2 \left(\mathbf{k} \cdot \mathbf{k}_* \geq \omega \right) \mathcal{T} \{ Q(\cdot; \omega) \tilde{u}(\mathbf{k}; \omega) \}(\mathbf{k}) \\
 & = 2 \left(\mathbf{k} \cdot \mathbf{k}_* \geq \omega \right) \mathcal{T} \{ Q(\cdot; \omega) \tilde{u}(\mathbf{k}; \omega) \}(\mathbf{k}) \\
 & + \mathcal{T} \{ R[\mathbf{k}; \omega] \}(\mathbf{k}), \quad b = 0, 1, 2, \dots
 \end{aligned}$$

Therefore, $D\tilde{G}[0, 0, \cdot, \cdot] = I$ is invertible. Note that we use the fact that $0 < r < 1$ to conclude that $\lim_{\epsilon \rightarrow 0} \epsilon^{-2} (\cdot \geq \cdot_*) \wedge [E(\cdot) - E - 2e] \equiv 0$. The implicit function theorem implies that there exists $\epsilon_0 > 0$ and a unique $\tilde{G} : [\cdot, \cdot] \in \mathcal{X}^2$ satisfying

$$(5.18) \quad \tilde{G}(\tilde{G}[\cdot, \cdot], \cdot, \cdot) = 0$$

for $0 < \epsilon < \epsilon_0$.

Equation (5.18) is equivalent to

$$(5.19) \quad \tilde{G}(\cdot) = \frac{\mathcal{T} \left(Q(\cdot) - (\cdot) R[\cdot, \cdot] \right)}{E(\cdot) - E - 2e}.$$

We now demonstrate the inequality in (5.13). Using (2.18), (5.11), and the invertibility of $L - 2e$, we obtain

$$(5.20) \quad \begin{aligned} \|\cdot\|_{2(\mathbb{R}^d)} &\leq C \|\tilde{G}(\cdot)\|_{\mathcal{X}^2} \\ &= 2C \frac{\|(\cdot \geq \cdot_*) \mathcal{T} \{Q(\cdot) - (\cdot) R[\cdot, \cdot]\}(\cdot)\|_{\mathcal{X}^2}}{\|E(\cdot) - E - 2e\|_{\mathcal{X}^2}} \\ &\leq 2^{-2} C \frac{(1 + b^2) \mathcal{T} \{Q(\cdot) - (\cdot) R[\cdot, \cdot]\}(\cdot)}{1 + b^2} \\ &\leq 2^{-2} C \|Q(\cdot) - (\cdot) R[\cdot, \cdot]\|_{2(\mathbb{R}^d)} \\ &\leq 2^{-2} C (1 + \epsilon^{-1}) \|\cdot\|_{2(\mathbb{R}^d)} + \|\cdot\|_{2(\mathbb{R}^d)} + 1 + \epsilon, \end{aligned}$$

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 $2^{-2} C \leq 1/2$, we can subtract the term involving $2^{-2} C \|\cdot\|_{2(\mathbb{R}^d)}$ from both sides of the inequality and then divide by $1 - 2^{-2} C(1 + \epsilon^{-1})$ to obtain the desired estimate (5.13). \square

Remark 5.2. Note that we do not obtain smoothness of \tilde{G} in \mathcal{X} . When applying the implicit function theorem in the above proof, we did not use any smoothness of the map \tilde{G} in \mathcal{X} . This is because of the sharp, ϵ -dependent cutoff function $(\cdot \geq \cdot_*)$.

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

5.2. Near frequency equation (5.10) with the aid of certain Taylor expansions for $\epsilon < \epsilon_0$, where we invoke our regularity hypothesis H1:

$$(5.21) \quad \begin{aligned} E_*(\cdot) &= E + \frac{1}{2} \sum_{j,l} E_{*jl}(\cdot) k_j k_l + \frac{1}{6} \sum_{j,l,m} E_{*jlm}(\cdot) k_j k_l k_m \\ &= E + A(\cdot) k k + \frac{1}{6} \sum_{j,l,m} E_{*jlm}(\cdot) k_j k_l k_m, \\ \rho_*(\cdot; \cdot) &= \rho_*(\cdot; 0) + \sum_j \rho_{*j}(\cdot; \cdot) k_j \\ &= w(\cdot) + \end{aligned}$$

for some

Lemma 5.2.

(A) Assume $\tilde{\rho}_{near}(\cdot)$ is given by (5.28). Then

$$A \frac{k}{\cdot} \frac{k}{\cdot} e^{-\tilde{\rho}_{near}(\cdot)} = \mathcal{F}_y A \cdot_j \cdot_l e^{-\rho(\cdot)} \quad (\cdot < -1) - .$$

(B)

(5.29)

$$\mathcal{T}_* \{Q(\cdot) \tilde{\rho}_{near}(\cdot)\}(\cdot) = \frac{1}{\mathcal{F}_y} Q(\cdot \leq -1) - + \mathcal{E}(\cdot),$$

where

$$(5.30) \quad \mathcal{E} \in L^2(\mathbb{R}^d) \leq C \quad Q \in L^s(\mathbb{R}^d) \quad L^2(\mathbb{R}^d),$$

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

Proof of Lemma 5.2. Recall the notation $\mathcal{F}f = \hat{f}$ for the Fourier transform given by (1.3). By (5.28) since $\tilde{\rho}_{near}$ is localized near 0 we have, Taylor expanding $\rho_*(\cdot; \cdot)$ about $\cdot = 0$,

$$\begin{aligned} \rho_*(\cdot; \cdot) &= \rho_*(\cdot; 0) \mathcal{F}^{-1} \left(\cdot < \cdot \right) \frac{1}{\cdot} \cdot \cdot (\cdot) + \mathcal{E}_1(\cdot) \\ &= \rho_*(\cdot; 0) \cdot_y < -1 (\cdot)_y \cdot_x + \mathcal{E}_1(\cdot), \\ \mathcal{E}_1 \in L^2(\mathbb{R}^d) &\leq C \in L^2(\mathbb{R}^d), \quad C = C \quad \mathbf{k} \rho_* \in \infty(\Omega \times \Omega^*)^d \cdot \end{aligned}$$

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

$$(5.31) \quad \begin{aligned} \mathcal{T}\{Q(\cdot) \tilde{\rho}_{near}(\cdot)\}(\cdot, \cdot) \\ = \rho_*(\cdot; 0) \mathcal{T}\{Q(\cdot)\}(\cdot, \cdot) < -1 (\cdot) (\cdot, \cdot) + \mathcal{T}\{Q(\cdot)\mathcal{E}_1(\cdot)\}(\cdot, \cdot). \end{aligned}$$

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

$$(5.32) \quad \begin{aligned} \mathcal{T}\{Q(\cdot)\}(\cdot, \cdot) < -1 (\cdot) (\cdot, \cdot) \\ = \mathcal{F}_x \{Q(\cdot)\}(\cdot) < r^{41} (\cdot) (\cdot) \\ + \\ \mathbf{m} \end{aligned}$$

the sum can be estimated as follows:

$$\int_{|\mathbf{m}| \leq 1} Q -$$

The right-hand side has the form

$$\begin{aligned}
 \mathcal{F}H[\psi, \phi, \eta] &= (\kappa < -1)(\tilde{R}_{near}[(\kappa < -1) / \psi, \phi] + \tilde{R}[\eta]) \\
 (5.41) \quad &= (\kappa < -1) \left(F(\kappa) + w(\cdot), U^\#(\cdot, \kappa) \right)_{2(\Omega)} \\
 &\quad + \mathcal{O}(\|\psi\|^{2-2\epsilon} + \|\phi\|^{3-2\epsilon}).
 \end{aligned}$$

We define the operators $\mathcal{L}, \mathcal{M} :$

$$(5.42) \quad \mathcal{L} \equiv (\psi < -1), \quad \mathcal{M} \equiv 1 - \mathcal{L} = (\psi \geq -1).$$

In physical space we can write (5.40) as

$$(5.43) \quad L \begin{pmatrix} \psi \\ \phi \\ \eta \end{pmatrix} = H[\psi, \phi, \eta],$$

where

$$\begin{aligned}
 (5.44) \quad H[\psi, \phi, \eta](x) &= F(\kappa) + w(\cdot), U^\#(\cdot, \kappa) \Big|_{2(\Omega)} + h[\psi, \phi, \eta], \\
 h[\psi, \phi, \eta] \Big|_{2(\mathbb{R}^d)} &\leq C(\|\psi\|^{2-2\epsilon} + \|\phi\|^{3-2\epsilon})(1 + \|\eta\|_{2(\mathbb{R}^d)}).
 \end{aligned}$$

In order to solve (5.43), we require a regularization that guarantees the invertibility of the operator L . Since zero is an isolated eigenvalue of L , there is a small disc of radius ϵ about zero, with boundary C_ρ such that for sufficiently small ϵ , C_ρ encircles m eigenvalues of L , counting multiplicity, where m is the multiplicity of zero as an eigenvalue of L .

Introduce the projection onto the spectral subspace associated with eigenvalues of L , encircled by C_ρ :

$$(5.45) \quad \mathcal{P} \equiv \frac{1}{2\pi i} \int_{C_\rho} (L - \lambda I)^{-1} d\lambda.$$

Note that

$$(5.46) \quad \mathcal{P} 0 = \langle F(\cdot), \cdot \rangle_{2(\mathbb{R}^d)}$$

projects onto the kernel of L .

We now rewrite (5.43) as the following system for ψ and η :

$$(5.47) \quad L \begin{pmatrix} \psi \\ \eta \end{pmatrix} = (I - \mathcal{P}) H[\psi, \phi, \eta],$$

$$(5.48) \quad H[\psi, \phi, \eta] = 0.$$

Any solution (ψ, η) of (5.47), (5.48) is a solution of (5.43).

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

$$(5.49) \quad \psi = (L - \mathcal{P})^{-1} (I - \mathcal{P}) \left(F + w(\cdot), U^\#(\cdot, \kappa) \right)_{2(\mathbb{R}^d)} + h[\psi, \phi, \eta].$$

Indeed, the solution may be constructed using the iteration

$$\begin{aligned}
 (5.50) \quad \psi_{+1} &= (L - \mathcal{P})^{-1} (I - \mathcal{P}) \left(F + w(\cdot), U^\#(\cdot, \kappa) \right)_{2(\mathbb{R}^d)} + h[\psi, \phi, \eta], \\
 \psi_0 &= (L - \mathcal{P})^{-1} (I - \mathcal{P}) \left(F + w(\cdot), U^\#(\cdot, \kappa) \right)_{2(\mathbb{R}^d)}.
 \end{aligned}$$

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

+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 $M(E)$

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

$$(A.13) \quad L e^{2\pi i k_* \cdot x} f(x) = e^{2\pi i k_* \cdot x} L^{(k_*)} f(x)$$

implies

$$(A.14) \quad e^{2\pi i k_* \cdot x} L^{(k_*)^{-1}} \{(\cdot + 2ik_*)p_*(\cdot; \cdot)\}(x) = L^{-1} \{(\cdot + 2ik_*)p_*(\cdot; \cdot)\}(x),$$

and the result follows.

A B. H **a a a a a a a**. 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

$$(B.1) \quad \mathcal{E}[u] = \int_{\mathbb{R}^d}$$

