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DEFECT MODES AND HOMOGENIZATION OF PERIODIC SCHRODINGER OPERATORS

M. A. HOEFER[†] M. I. WEINSTEIN[‡]

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

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

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Our results concern a particular class of weak defects, slowly varying and of small amplitude: $\varepsilon^2 Q(\varepsilon\ )$*, 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,* $\varepsilon^2 Q(\varepsilon\ )$*, 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 e ective 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. N a a . We note that we may, without loss of generality, restrict ourselves to the case where the fundamental period cell is $\Omega = [0,1]$. Indeed, let $\mathcal{B}$ denote the fundamental period cell, spanned by the linearly independent vectors $\{\ _1, \ldots,\ \}$ and define the constant matrix $\mathcal{R}^{-1}$ to be the matrix whose jth column is . Then, under the change of coordinates $\ \mapsto\ = \mathcal{R}\ $,

$$-\nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{x}} + V(\ ) \text{ acting on } L^2\ (\mathcal{B}) \text{ transforms to}$$

$$-\nabla_{\mathbf{z}} \cdot \alpha\, \nabla_{\mathbf{z}} + \tilde{V}(\ ) \equiv -\sum_{1} \alpha\ \frac{\partial^2}{\partial z\, \partial z} + \tilde{V}(\ )$$

acting on $L^2\ [0,1]$, where

$$\alpha = \mathcal{R}\mathcal{R}\ ,\quad \tilde{V}(\ ) = V\ \mathcal{R}^{-1}\ ,\quad = \mathcal{R}^{-1}\ .$$

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

$$\mathcal{F}\{f\}(\ ) \equiv \hat{f}(\ ) = \int e^{-2\pi\ \mathbf{k}\cdot\mathbf{x}} f(\ )d\ , \tag{1.3}$$

$$\mathcal{F}^{-1}\{g\}(\ ) \equiv \check{g}(\ ) = \int e^{2\pi\ \mathbf{x}\cdot\mathbf{k}} g(\ )d\ .$$

   Thus, $\mathcal{F}\,\mathcal{F}^{-1} = \mathrm{Id}$.
3. $\Omega = [0,1]$ is the fundamental period cell; $\Omega\ = [-1/2, 1/2]$ is the dual fundamental cell or Brillouin zone.
4. 1 (

6. Fourier spectral cuto :

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We will study the bifurcation of eigenvalues from the band edge

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

with the associated, real-valued band edge eigenfunction

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

For example, the lowest band edge is $E_0(0)$ and the associated eigenfunction is periodic $p_0(\quad +$

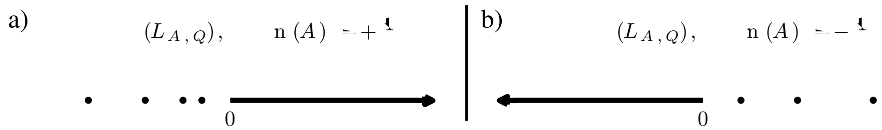

Fig. 3.1. *Discrete and continuous spectrum of* $L_{A,Q}$. (a) *Positive definite e ective mass tensor.* (b) *Negative definite e ective mass tensor.*

Set sgn(A) = +1 if A is positive definite and sgn(A) = −1 if A is negative definite. Assume L has a simple eigenvalue e with sgn(A)e < 0 and corresponding eigenfunction

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

$$\left\| u^{( )}(\cdot;\mu^{( )}) - \sum_{0} \varepsilon\, U^{( )}(\cdot,\varepsilon\cdot) \right\|_{2(\mathbb{R}^d)} \leq \varepsilon^{\ -1} C,$$

$$\left| \mu^{( )} - E - \varepsilon^2 e - \sum_{3} \varepsilon\, \mu^{( )} \right| \leq \varepsilon^{\ +1} C \tag{3.5}$$

for $j = 1, 2, \ldots, M$, 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. H a a a a . 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 $u\ (\ ;\mu\ )$ satisfies (1.1),

$$[-\Delta + V(\ ) + \varepsilon^2 Q(\varepsilon\ )]u = \mu\, u\ , \tag{4.1}$$

and expand it in an asymptotic series as follows:

$$u\ (\ ;\mu\ ) = U_\epsilon(\ ,\ ) = \sum_{0}^{\infty} \varepsilon\ U\ (\ ,\ ), \quad \mu = E + \sum_{1}^{\infty} \varepsilon\ \mu\ , \tag{4.2}$$

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

(4.3)

Viewed as a system of partial di erential 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

$$L \;\; U_2 = 2\partial_{\cdot\, j} F_1 \partial_{\cdot\, j} w - \mathcal{L}[F_0], \tag{4.16}$$

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

$$\begin{aligned} \mathcal{L}[G](\;,\;) = & -4\partial_{\cdot\, j} L^{-1}\{\partial_{\cdot\, l} w\}(\;)\partial_{\cdot\, j}\partial_{\cdot\, l} G(\;) \\ & + w(\;)[-\Delta_{\mathbf{y}} + Q(\;) - \mu_2]G(\;). \end{aligned} \tag{4.17}$$

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

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

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

$$A \;\; \equiv \delta \;\; - 4 \left\langle \partial_{\cdot\, j} w, L^{-1}\{\partial_{\cdot\, l} w\} \right\rangle_{\;\,2(\Omega)}. \tag{4.19}$$

Proposition 4.4.

$$A \;\; = \frac{1}{8\pi^2}\partial_{\;\, j}\partial_{\;\, l} E_{\;\, *}(\;\;). \tag{4.20}$$

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

Applying Proposition 4.1 to (4.16) gives

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

which is the e ective, homogenized equation for (1.1) with the e ective mass tensor A. We have assumed in H3 the existence of the eigenpair $F \;\; \in H^2(\mathbb{R} \;)$ and $e \;\; \in \mathbb{R} \setminus \{0\}$. Thus, $F_0(\;) = F \;\; (\;)$.

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

$$U_2(\;,\;) = w(\;)F_2(\;) + 2\partial_{\cdot\, j} F_1(\;) L^{-1}\{\partial_{\cdot\, j} w\}(\;) + L^{-1}\{\mathcal{L}[F \;\;](\cdot, \;)\}(\;). \tag{4.22}$$

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

$$L \;\; U_3 = 2\partial_{\cdot\, j} F_2 \partial_{\cdot\, j} w - \mathcal{L}[F_1] - \mathcal{H}_3 + \mu_3 w F \;\;, \tag{4.23}$$

where $\mathcal{H}_3$ is known:

$$\begin{aligned} \mathcal{H}_3(\;,\;) = & -2\partial_{\cdot\, j}\partial_{\cdot\, j} L^{-1}\{\mathcal{L}[F \;\;](\cdot, \;)\}(\;) \\ & + 2L^{-1}\{\partial_{\cdot\, j} w\}(\;)[-\Delta_{\mathbf{y}} + Q(\;) - e \;\;]\partial_{\cdot\, j} F(\;). \end{aligned} \tag{4.24}$$

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

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

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

$$\mu_3 = \left\langle F \;\; (\cdot), \langle w(\circ), \mathcal{H}_3(\circ, \cdot)\rangle_{\;\,2(\Omega)} \right\rangle_{\;\,2(\mathbb{R}^d)}. \tag{4.26}$$

We can now write F_1 in terms of F as

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

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

$$\begin{aligned} U_3(\ , \ ) &= w(\ )F_3(\ ) + 2\partial_{\ j} F_2(\ ) L^{-1}\{\partial_{\ j} w\}(\ ) \\ &\quad - L^{-1} \quad \mathcal{L}[F_1](\cdot, \ ) + \mathcal{H}_3(\cdot, \ ) - \mu_3 w(\cdot) F \quad (\ ) \quad (\ ), \end{aligned} \tag{4.28}$$

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

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

$$L \ U \ = 2\partial_{\ j} F_{\ -1} \partial_{\ j} w - \mathcal{L}[F_{\ -2}] - \mathcal{H} \ + \mu \ wF \ , \tag{4.29}$$

where $\mathcal{H}$

edge and “far” from the band edge:

$$
\begin{aligned}
&\Psi\ (\ ) = \Psi\quad (\ ) + \Psi\quad (\ ) = \mathcal{T}^{-1}\tilde{\Psi}\quad (\ ;\cdot) + \mathcal{T}^{-1}\tilde{\Psi}\quad (\ ;\cdot),\\
&\tilde{\Psi}\quad (\ ;\ ) = \Pi\quad \Psi\ (\ ) \equiv \chi(|\ \ -\ \ | < \varepsilon\ )\mathcal{T}_{*}\{\Psi\ \}(\ )p_{*}(\ ;\ ),\\
&\tilde{\Psi}\quad (\ ;\ ) = \Pi\quad \Psi\ (\ ) \equiv \sum_{0}^{\infty} \chi(|\ \ -\ \ | \geq \varepsilon\ \delta_{*}\ )\mathcal{T}\{\Psi\ \}(\ )p\ (\ ;\ ),
\end{aligned} \tag{5.5}
$$

where δ is the Kronecker delta function and the indicator functions are defined as

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

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

We will use the conventions

$$
\begin{aligned}
&\tilde{\Psi}\quad (\ ) \equiv \left\langle p_{*}(\cdot;\ ), \tilde{\Psi}\quad (\cdot;\ )\right\rangle_{\ ^{2}(\Omega)},\\
&\tilde{\Psi}\quad (\ ) \equiv \left\{\left\langle p\ (\cdot;\ ), \tilde{\Psi}\quad (\cdot;\ )\right\rangle_{\ ^{2}(\Omega)}\right\}_{\geq 0},
\end{aligned} \tag{5.7}
$$

where $\tilde{\Psi}\quad (\ )$ is a scalar and $\tilde{\Psi}\quad (\ )$ 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 $p\ (\cdot;\ )$, and use the properties (2.3) and (2.4) to find

$$
\begin{aligned}
&[E\ (\ ) - E\ \ - \varepsilon^{2}e\quad]\mathcal{T}\ \{\Psi\ \}(\ ) + \varepsilon^{2}\mathcal{T}\ \{Q(\varepsilon\cdot)\Psi\ (\cdot)\}(\ )\\
&\quad = \varepsilon^{2}\mathcal{T}\ \{R\ [\Psi\ , \mathrm{Y}\ ]\}(\ ),\quad b = 0, 1, \ldots.
\end{aligned} \tag{5.9}
$$

We view this as a coupled system of equations for the near and far frequency components $\tilde{\Psi}\quad (\ )$ and $\tilde{\Psi}\quad (\ )$, $\ \in \Omega\ $:

$$
\text{near:}\quad
\begin{cases}
(E_{*}(\ ) - E\ \ - \varepsilon^{2}e\quad)\tilde{\Psi}\quad (\ )\\
\quad + \varepsilon^{2}\chi(|\ \ | < \varepsilon\ )\mathcal{T}_{*}\{Q(\varepsilon\cdot)\Psi\quad (\cdot)\}(\ )\\
\quad = \varepsilon^{2}\chi(|\ \ | < \varepsilon\ )\Big[- \mathcal{T}_{*}\{Q(\varepsilon\cdot)\Psi\quad (\cdot)\}(\ )\\
\quad + \mathcal{T}_{*}\{R\ [\Psi\quad + \Psi\quad , \mathrm{Y}\ ]\}(\ )\Big],
\end{cases} \tag{5.10}
$$

$$
\text{far:}\quad
\begin{cases}
(E\ (\ ) - E\ \ - \varepsilon^{2}e\quad)\chi(|\ \ | \geq \varepsilon\ \delta_{*}\ )\tilde{\Psi}\quad (\ )\\
\quad + \varepsilon^{2}\chi(|\ \ | \geq \varepsilon\ \delta_{*}\ )\mathcal{T}\ \{Q(\varepsilon\cdot)\Psi\quad (\cdot)\}(\ )\\
\quad = \varepsilon^{2}\chi(|\ \ | \geq \varepsilon\ \delta_{*}\ )\Big[- \mathcal{T}\ \{Q(\varepsilon\cdot)\Psi\quad (\cdot)\}(\ )\\
\quad + \mathcal{T}\ \{R\ [\Psi\quad + \Psi\quad , \mathrm{Y}\ ]\}(\ )\Big],\quad b = 0, 1, 2, \ldots.
\end{cases} \tag{5.11}
$$

Therefore, $D\tilde{G}[0, 0, \psi, \upsilon] = I$ is invertible. Note that we use the fact that $0 < r < 1$ to conclude that $\lim_{\to 0} \varepsilon^2 \chi(| \ | \geq \varepsilon \ \delta_*)/[E(\ ) - E \ - \varepsilon^2 e \ ] \equiv 0$. The implicit function theorem implies that there exists $\varepsilon_0 > 0$ and a unique $\tilde{\Psi} \ [\Psi \ , \Upsilon \ ] \in \mathcal{X}^2$ satisfying

$$\tilde{G} \ \tilde{\Psi} \ [\Psi \ , \Upsilon \ ], \varepsilon, \Psi \ , \Upsilon \ = 0 \tag{5.18}$$

for $0 < \varepsilon < \varepsilon_0$.

Equation (5.18) is equivalent to

$$\tilde{\Psi} \ (\ ) = -\varepsilon^2 \frac{\mathcal{T} \ \Pi \ Q(\varepsilon\cdot)\Psi \ (\cdot) - R \ [\Psi \ + \Psi \ , \Upsilon \ ](\cdot) \ (\ )}{E(\ ) - E \ - \varepsilon^2 e}. \tag{5.19}$$

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

(5.20)

$$\begin{aligned} \|\Psi \ \|_{2(\mathbb{R}^d)} &\leq C \ \tilde{\Psi} \ _{X^2} \\ &= \varepsilon^2 C \ \frac{\chi(|\cdot| \geq \varepsilon \ \delta_*)\mathcal{T}\{Q(\varepsilon\circ)\Psi \ (\circ) - R \ [\Psi \ , \Upsilon \ ](\circ)\}(\cdot)}{E(\cdot) - E \ - \varepsilon^2 e} \ _{X^2} \\ &\leq \varepsilon^{2-2} \ C \ \frac{(1+b^2 \ )\mathcal{T}\{Q(\varepsilon\circ)\Psi \ (\circ) - R \ [\Psi \ , \Upsilon \ ](\circ)\}(\cdot)}{1+b^2} \ _{X^0} \\ &\leq \varepsilon^{2-2} \ C \ \|Q(\varepsilon\cdot)\Psi \ (\cdot) - R \ [\Psi \ , \Upsilon \ ](\cdot)\|_{2(\mathbb{R}^d)} \\ &\leq \varepsilon^{2-2} \ C \ (1 + \varepsilon^{\ -1}\Upsilon \ ) \ \|\Psi \ (\cdot)\|_{2(\mathbb{R}^d)} + \|\Psi \ (\cdot)\|_{2(\mathbb{R}^d)} \ + 1 + \Upsilon \ , \end{aligned}$$

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

Remark 5.2. Note that we do not obtain smoothness of Ψ 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 cuto function $\chi(| \ | \geq \varepsilon \ )$.

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

5.2. N a a a a . We now study the near frequency equation (5.10) with the aid of certain Taylor expansions for $| \ | < \varepsilon$, where we invoke our regularity hypothesis H1:

$$\begin{aligned} E_*(\ ) &= E \ + \frac{1}{2}\partial_j\partial_l E_*(0)k \ k \ + \frac{1}{6}\partial_j\partial_l\partial_m E_*(\ )k \ k \ k \\ &= E \ + A \ k \ k \ + \frac{1}{6}\partial_j\partial_l\partial_m E_*(\ )k \ k \ k \ , \\ p_*(\ ; \ ) &= p_*(\ ; 0) + \partial_j p_*(\ ; \ )k \\ &= w(\ ) + \partial \end{aligned} \tag{5.21}$$

for some

Lemma 5.2.

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

$$A\ \frac{k}{\varepsilon}\ \frac{k}{\varepsilon} - e \qquad \tilde{\Psi}_{near}(\ )$$
$$= \mathcal{F}_{\mathbf{y}}\ \ A\ \ \partial_{\cdot\ j}\partial_{\cdot\ l} - e \qquad \chi(|\nabla| < \varepsilon^{\ -1})\ \Phi \quad \overline{\varepsilon}\ .$$

(B)

$$\mathcal{T}_{*}\{Q(\varepsilon\cdot)\Psi_{near}(\cdot)\}(\ ) = \frac{1}{\varepsilon}\mathcal{F}_{\mathbf{y}}\ \ Q\ \chi(|\nabla| \leq \varepsilon^{\ -1})\Phi \quad \overline{\varepsilon} \ + \ \mathcal{E}(\ ), \tag{5.29}$$

where

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

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

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

$$\Psi\qquad(\ ) = p_{\ *}(\ ;0)\ \mathcal{F}^{-1}\quad \chi(|\cdot| < \varepsilon\ )\ \frac{1}{\varepsilon}\ \Phi\ \ \frac{\cdot}{\varepsilon}\qquad(\ )\ +\ \mathcal{E}_1(\ )$$
$$= p_{\ *}(\ ;0)\chi\ \ |\nabla_{\mathbf{y}}| < \varepsilon^{\ -1}\ \ \Phi(\ )|_{\mathbf{y}\ \ \mathbf{x}} + \mathcal{E}_1(\ ),$$
$$\|\mathcal{E}_1\|_{\ ^2(\mathbb{R}^d)} \leq C\varepsilon\ \|\Phi\|_{\ ^2(\mathbb{R}^d)}, \qquad C = C\ \ \|\nabla_{\mathbf{k}}p_{\ *}\|_{\ ^\infty(\Omega\times\Omega^*)^d}\ .$$

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

$$\begin{aligned}&\mathcal{T}\{Q(\varepsilon\cdot)\Psi\qquad(\cdot)\}(\ ,\ \ )\\ &= p_{\ *}(\ ;0)\ \mathcal{T}\ \ Q(\varepsilon\cdot)\ \chi\ \ |\nabla_{\ \cdot}| < \varepsilon^{\ -1}\ \ \Phi(\varepsilon\cdot)\ \ (\ ,\ \ ) + \mathcal{T}\{Q(\varepsilon\cdot)\mathcal{E}_1(\cdot)\}(\ ,\ \ ).\end{aligned} \tag{5.31}$$

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

$$\begin{aligned}&\mathcal{T}\ \ Q(\varepsilon\cdot)\ \chi\ \ |\nabla_{\ \cdot}| < \varepsilon^{\ -1}\ \ \Phi(\varepsilon\cdot)\ \ (\ ,\ \ )\\ &= \mathcal{F}_{\mathbf{x}}\ \ Q(\varepsilon\cdot)\ \chi\ \ |\nabla_{\ \cdot}| < \varepsilon^{r\ -1}\ \ \Phi(\varepsilon\cdot)\ \ (\ )\\ &+ \\ &\quad \mathbf{m}\end{aligned} \tag{5.32}$$

the sum can be estimated as follows:

$$\sum_{|\mathbf{m}|\geq 1} \int \left| Q \quad \frac{\quad}{\varepsilon} \quad \right|$$

The right-hand side has the form

$$\begin{aligned}\mathcal{F}H[\Phi, \Upsilon, \varepsilon] &= \chi(|\kappa| < \varepsilon^{-1})(\varepsilon\ \tilde{R}_{near}[\chi(|\nabla| < \varepsilon^{-1})\Phi/\varepsilon, \Upsilon] + \tilde{R}[\Phi]) \\ &= \chi(|\kappa| < \varepsilon^{-1})\ \Upsilon\ F(\kappa) + \langle w(\cdot), U^{\#}(\cdot, \kappa)\rangle_{L^2(\Omega)} \\ &\quad + \mathcal{O}(\varepsilon + \varepsilon^{2-2} + \varepsilon^{3-2}) .\end{aligned} \tag{5.41}$$

We define the operators χ, $\overline{\chi}$:

$$\chi \equiv \chi(|\nabla_{\mathbf{y}}| < \varepsilon^{-1}), \quad \overline{\chi} \equiv 1 - \chi = \chi(|\nabla_{\mathbf{y}}| \geq \varepsilon^{-1}). \tag{5.42}$$

In physical space we can write (5.40) *as*

$$\chi L \chi \Phi = \chi H[\Phi, \Upsilon, \varepsilon], \tag{5.43}$$

where

$$\begin{aligned} H[\Phi, \Upsilon, \varepsilon]() &= \Upsilon F() + \langle w(\cdot), U^{\#}(\cdot,)\rangle_{L^2(\Omega)} + h[\Phi, \Upsilon, \varepsilon], \\ \|\chi h[\Phi, \Upsilon, \varepsilon]\|_{L^2(\mathbb{R}^d)} &\leq C(\varepsilon + \varepsilon^{2-2} + \varepsilon^{3-2})(1 + \|\Phi\|_{L^2(\mathbb{R}^d)}).\end{aligned} \tag{5.44}$$

In order to solve (5.43), we require a regularization that guarantees the invertibility of the operator $\chi L \chi$. Since zero is an isolated eigenvalue of L, there is a small disc of radius $\rho = \rho$ about zero, with boundary C_ρ such that for ε sufficiently small, C_ρ encircles m eigenvalues of $\chi L \chi$, 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 $\chi L \chi$, encircled by C_ρ:

$$\Pi \equiv \frac{1}{2\pi i}\int_{C_\rho} (\chi L \chi - \lambda I)^{-1}\, d\lambda. \tag{5.45}$$

Note that

$$\Pi_0 = \langle F, \cdot \rangle_{L^2(\mathbb{R}^d)} \tag{5.46}$$

projects onto the kernel of L.

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

$$\chi L \chi \Phi = \chi (I - \Pi)\chi H[\Phi, \Upsilon, \varepsilon], \tag{5.47}$$

$$\chi \Pi \chi H[\Phi, \Upsilon, \varepsilon] = 0. \tag{5.48}$$

Any solution (Φ, Υ) of (5.47), (5.48) is a solution of (5.43).

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

$$\Phi = (\chi L \chi)^{-1} (I - \Pi) \left[\Upsilon F + \langle w(\cdot), U^{\#}(\cdot,)\rangle_{L^2(\mathbb{R}^d)} + h[\Phi, \Upsilon, \varepsilon]\right]. \tag{5.49}$$

Indeed, the solution may be constructed using the iteration

$$\begin{aligned}\Phi_{+1} &= (\chi L \chi)^{-1}\chi (I - \Pi)\chi \left[\Upsilon F + \langle w(\cdot), U^{\#}(\cdot,)\rangle_{L^2(\mathbb{R}^d)} + h[\Phi, \Upsilon, \varepsilon]\right], \\ \Phi_0 &= (\chi L \chi)^{-1}\chi (I - \Pi) \left[\Upsilon F + \langle w(\cdot), U^{\#}(\cdot,)\rangle_{L^2(\mathbb{R}^d)}\right].\end{aligned} \tag{5.50}$$

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

$\|\Phi_{+1} - \Phi$

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

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

implies

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

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

$$\mathcal{E}[u] = \int_{\mathbb{R}} \tag{B.1}$$