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DEFECT MODES AND HOMOGENIZATION OF PERIODIC SCHRODINGER OPERATORS

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Ab ac . We consider the discrete eigenvalues of the operator $H_\varepsilon = -\Delta + \ (\ ) + \varepsilon^2 \ (\varepsilon\ )$, where ( ) is periodic and ( ) 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 Schr¨

6. Fourier spectral cuto :

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We will study the bifurcation of eigenvalues from the band edge

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

with the associated, real-valued band edge eigenfunction

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

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

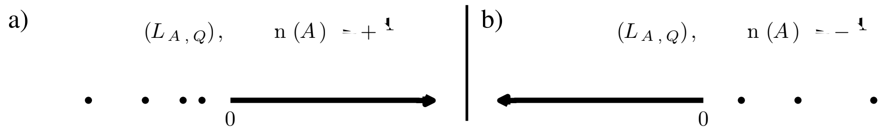

Fig. 3.1. *Discrete and continuous spectrum of* $L_{A,Q}$. (a) *Positive definite e ective mass tensor.* (b) *Negative definite e ective mass tensor.*

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

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

$$\left| \mu^{( )} \quad E \quad \varepsilon^2 e \quad \varepsilon\, \mu^{( )} \right| \le \varepsilon^{\;+1} C \tag{3.5}$$

for $j = 1, 2, \ldots, M$, all $N \ge 4$, 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),

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

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

(4.16)
$$L\ U_2 = 2\partial_{\cdot j} F_1 \partial_{\cdot j} w \quad \mathcal{L}[F_0],$$

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

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

Definition 4.3. *Define the operator* L : H^2

We can now write F_1 in terms of F as

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

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

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

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

$$L \; U \; = 2\partial_{\cdot\, j} F \;_{-1} \partial_{\cdot\, j} w \quad \mathcal{L}[F \;_{-2}] \quad \mathcal{H} \; + \mu \; wF \quad , \tag{4.29}$$

where $\mathcal{H}$

edge and “far” from the band edge:

(5.5)
$$\Psi\,(\ ) = \Psi\quad(\ ) + \Psi\ (\ ) = \mathcal{T}^{-1}\tilde{\Psi}\quad(\ ;\cdot) + \mathcal{T}^{-1}\tilde{\Psi}\ (\ ;\cdot),$$
$$\tilde{\Psi}\quad(\ ;\ ) = \Pi\quad\Psi\,(\ ) \equiv \chi(\qquad < \varepsilon\ )\mathcal{T}_{\ast}\{\Psi\ \}(\ )p_{\ast}(\ ;\ ),$$
$$\tilde{\Psi}\ (\ ;\ ) = \Pi\ \ \Psi\,(\ ) \equiv \sum_{0}^{\infty} \chi(\qquad \geq \varepsilon\ \delta_{\ast}\ )\mathcal{T}\{\Psi\ \}(\ )p\ (\ ;\ ),$$

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

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

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

(5.7)
$$\tilde{\Psi}\quad(\ ) \equiv \left\langle p_{\ast}(\cdot;\ ), \tilde{\Psi}\quad(\cdot;\ )\right\rangle_{2(\Omega)},$$
$$\tilde{\Psi}\ (\ ) \equiv \left\{\left\langle p\ (\cdot;\ ), \tilde{\Psi}\ (\cdot;\ )\right\rangle_{2(\Omega)}\right\}_{\geq 0},$$

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

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

the choice of which will be made clear later.

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

(5.9)
$$[E\ (\ )\quad E\quad \varepsilon^{2}e\quad]\mathcal{T}\ \{\Psi\ \}(\ ) + \varepsilon^{2}\mathcal{T}\ \{Q(\varepsilon\cdot)\Psi\ (\cdot)\}(\ )$$
$$= \varepsilon^{2}\mathcal{T}\ \{R\ [\Psi\ ,\Upsilon\ ]\}(\ ), \quad b = 0, 1, \ldots.$$

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

(5.10) near:
$$\begin{cases} (E_{\ast}(\ )\quad E\quad \varepsilon^{2}e\quad)\tilde{\Psi}\quad(\ ) \\ +\,\varepsilon^{2}\chi(\quad < \varepsilon\ )\mathcal{T}_{\ast}\{Q(\varepsilon\cdot)\Psi\quad(\cdot)\}(\ ) \\ = \varepsilon^{2}\chi(\quad < \varepsilon\ )\Big(\ \ \mathcal{T}_{\ast}\{Q(\varepsilon\cdot)\Psi\ \ (\cdot)\}(\ ) \\ +\,\mathcal{T}_{\ast}\{R\ [\Psi\quad + \Psi\ \ ,\Upsilon\ ]\}(\ )\Big), \end{cases}$$

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

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

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

for $0 < \varepsilon < \varepsilon_0$.

Equation (5.18) is equivalent to

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

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

$$\begin{aligned} \Psi \quad {}_{^2(\mathbb{R}^d)} &\leq C\ \tilde{\Psi} \quad {}_{\mathcal{X}^2} \\ &= \varepsilon^2 C\ \chi(\ \cdot\ \geq \varepsilon\ \delta_{\ *} \end{aligned}$$

for some

Lemma 5.2.

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

$$A \quad \frac{k}{\varepsilon} \ \frac{k}{\varepsilon} \quad e \qquad \tilde{\Psi}_{near}(\ )$$

$$= \mathcal{F}_{\mathbf{y}} \quad A \quad \partial_{\cdot\, j} \partial_{\cdot\, l} \quad e \qquad \chi$$

the sum can be estimated as follows:

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

The right-hand side has the form

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

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

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

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

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

where

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

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:

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

Note that

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

projects onto the kernel of L.

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

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

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

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:

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

Indeed, the solution may be constructed using the iteration

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

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

$\Phi_{+1} \quad \Phi$

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

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

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

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