

## 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  $\{b_1, \dots, b_d\}$  and define the constant matrix  $\mathcal{R}^{-1}$  to be the matrix whose  $j$ th column is  $b_j$ . Then, under the change of coordinates  $x \mapsto z = \mathcal{R}^{-1}x$ ,

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

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.  $1(x)$

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  $\rho_0(\mathbf{x})$ .



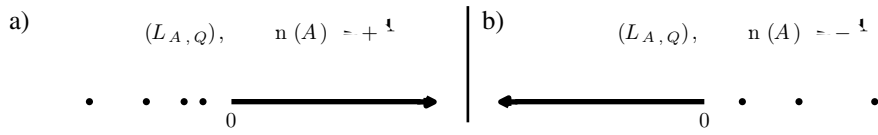


Fig. 3.1. Discrete and continuous spectrum of  $L_{A,Q}$ . (a) Positive definite effective mass tensor. (b) Negative definite effective mass tensor.

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  $L_\epsilon$ ). In spatial dimensions,  $d > 1$ , the operator  $L_\epsilon$  may have degenerate eigenvalues, e.g., if there is symmetry in  $Q(\cdot)$ . Suppose  $e_\epsilon$  has multiplicity  $M$ . Then, since  $L_\epsilon$  is self-adjoint,  $e_\epsilon$  perturbs, generically, to  $M$  distinct branches. Thus, applying the method of proof of Theorem 3.1, each degenerate eigenvalue of  $L_\epsilon$  of multiplicity  $M$  gives rise to  $M$  branches of eigenpairs of  $H_\epsilon$ . The cluster of  $M$  distinct eigenvalues of  $H_\epsilon$  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  $\epsilon$ . 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. ( $\epsilon^n$ )** **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  $\mathcal{H}$







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

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

for  $0 < \epsilon < \epsilon_0$ .

Equation (5.18) is equivalent to

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

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

$$\begin{aligned} \|\cdot\|_{2(\mathbb{R}^d)} &\leq C \|\cdot\|_{X^2} \\ &= C \|\cdot\|_{\geq \cdot_*} \end{aligned}$$



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  $\cdot = 0$ ,

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

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

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

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

$$(5.32) \quad \begin{aligned} \mathcal{T}\{Q(\cdot)\}(\cdot, \cdot) &\leq -1 \rho_*(\cdot) (\cdot, \cdot) \\ &= \mathcal{F}_x^{-1} Q(\cdot) \leq -1 \rho_*(\cdot) (\cdot) (\cdot) \\ &+ \\ &\mathbf{m} \end{aligned}$$

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  $\epsilon$  about zero, with boundary  $C_\rho$  such that for sufficiently small  $\epsilon$ ,  $C_\rho$  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  $C_\rho$ :

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

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  $\psi$  and  $\eta$ :

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

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

Any solution  $(\psi, \eta)$  of (5.47), (5.48) is a solution of (5.43).

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

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

Indeed, the solution may be constructed using the iteration

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

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  $2 \times 2$  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

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

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

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







