

DEFECT RESONANCES OF TRUNCATED CRYSTAL STRUCTURES*

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Abstract. Defects in the atomic structure of crystalline materials may spawn electronic bound states, known as *defect states*, which decay rapidly away from the defect. Simplified models of defect states typically assume the defect is surrounded on all sides by an infinite perfectly crystalline material. In reality the surrounding structure must be finite, and in certain contexts the structure can be small enough that edge effects are significant. In this work we investigate these edge effects and prove the following result. Suppose that a one-dimensional infinite crystalline material hosting a positive energy defect state is truncated a distance M from the defect. Then, for sufficiently large M , there exists a resonance *exponentially close* (in M) to the bound state eigenvalue. It follows that the truncated structure hosts a metastable state with an exponentially long lifetime. Our methods allow both the resonance frequency and associated resonant state to be computed to all orders in e^{-M} . We expect this result to be of particular interest in the context of photonic crystals, where defect states are used for wave-guiding and structures are relatively small. Finally, under a mild additional assumption we prove that if the defect state has negative energy, then the truncated structure hosts a bound state with exponentially close energy.

Key words. defect states, resonances, periodic structures, metastable states

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1. Introduction. In this work we seek to understand solutions of the following model PDE:

$$(1.1) \quad i\partial_t\psi = H\psi \quad H := D_x^2 + V(x), \quad D_x := -i\nabla_x.$$

Here $\psi(x, t) : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{C}$ is a complex function known as the wave-function, H is the Hamiltonian, and $V(x)$ is a real function known as the potential. The PDE (1.1) arises in two application areas which are relevant to the present work. First, (1.1) models the wave-like dynamics of electrons in a d -dimensional material in the independent-electron approximation (see, e.g., [3]). In this case, $\psi(x, t)$ denotes the wave-function of a single electron, and $V(x)$ denotes the electric potential due to the material environment. The other application area is in photonics, where the propagation of electromagnetic waves through media with spatially varying refractive index can be modeled in the paraxial approximation by (1.1) (see, e.g., [2]). In this case, $\psi(x, t)$ denotes the envelope of an electromagnetic wave-packet, and $V(x)$ is related to the refractive index of the medium.

In both of these application areas, there is considerable interest in building *wave-guides*: structures which effectively confine waves to a given region or channel. The

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simplest way to confine waves is by building a structure which hosts a bound state, as we now briefly review. Suppose H has a bound state, i.e., there exists $E \in \mathbb{R}$ and $\phi(x) \in L^2(\mathbb{R}^d)$ such that $H\phi = E\phi$. Then the solution of (1.1) with initial condition $\psi(x, 0) = \phi(x)$ is $\psi(x, t) = e^{-iEt}\phi(x)$. Since the magnitude of the solution $|\psi(x, t)|^2 = |\phi(x)|^2$ is conserved with respect to time, and since $\phi(x)$ spatially decays, stationary solutions describe waves which remain confined for all $t > 0$.

A common strategy for creating a structure which hosts a bound state is to build a structure which is perfectly periodic except for a defect region. Bound states created by defects in an otherwise periodic structure are known as *defect states*. Many previous works have proved existence of defect states across various models; see, e.g., [7, 9, 12, 22, 24, 32, 33, 35, 37, 41, 55]. For related numerical work, see [31, 56]. In recent years, “topologically protected” edge states, which decay away from the physical edge of a material, or away from extended line defects within a material, have also attracted attention for wave-guiding applications [18, 19, 20, 21, 28, 29, 30, 46]. For related numerical work, see [58].

In general these works make the unphysical assumption that the periodic structure surrounding the defect, edge, or line defect, extends infinitely away from the defect. It follows that these models capture the dynamics of real wave-guides only approximately. In this work we investigate the validity of this approximation by investigating how bound states of infinite periodic structures supporting a defect state perturb when the structure is truncated, i.e., when the potential $V(x)$ is set equal to zero outside a bounded region. Before we can state our result, we need to recall the basic theory of resonances (for more detail, see, e.g., [26]).

Resonances are poles of the resolvent $(H - z)^{-1}$ viewed as a function of $\lambda := \sqrt{z}$ and meromorphically continued to the lower half of the complex plane ($\text{Im } \lambda < 0$). For our purposes, resonances are important because they control the rate of energy decay of solutions of (1.1) from bounded subsets of \mathbb{R}^d . Specifically, suppose that H has a resonance z^* in the strip $0 < a \leq \text{Re } z \leq b$ whose imaginary part is closer to the real axis than any other resonance in that strip. Let $\chi_R \in C_c^\infty$ denote a smooth cutoff which equals one on $B(0, R)$ for some $R > 0$, and let $\psi \in C_c^\infty$ denote a cutoff with $\text{supp } \psi = [a, b]$. Then one can prove a bound (roughly stated, see, e.g., [8, 26] for more details)

$$(1.2) \quad \chi_R e^{-itH} \chi_R \psi(H) = \chi_R \text{Res} (e^{-it\bullet} (H - \bullet)^{-1}, z^*) \chi_R \psi(H) \\ + \text{terms decaying faster in time.}$$

It follows that the imaginary part of z^* controls the rate of decay of solutions of (1.1) localized spatially in the ball $B(0, R)$ and spectrally in the interval $[a, b]$.

The main result proved in this work is as follows. We prove that when an infinite structure hosting a defect state with positive energy $E > 0$ is truncated sufficiently far from the defect and $d = 1$, the truncated structure hosts a resonance exponentially close (in the distance from the defect to the truncation) in the complex plane to E . Furthermore, our methods allow for precise estimates of the exponentially small corrections to all orders.

As a corollary we prove precise estimates on the rate of decay of waves localized at defects in truncations of infinite one-dimensional structures hosting defect states with positive energy $E > 0$. This result clarifies the validity of the unphysical approximation described above, where wave-trapping by finite structures is studied using models which are periodic away from the defect. For the precise statement of our main result in the simplest setting where reflection symmetry holds, see section 2.

For the statement of our result in the general case where reflection symmetry may be broken, see section 7.

We hope that our result will inform the design of novel wave-guiding devices based on defect states. Another motivation and potential application of our result is to the design of efficient lasers. Lasers require the existence of a resonance very close to the real axis. Our work implies that truncations of infinite structures which host defect states with positive energy will lase efficiently if they are truncated sufficiently far from the defect. In recent years “topological” lasers, whose associated resonances arise because of edge modes, have been proposed and built [4, 36, 54, 57, 61].

By adapting our methods we can prove one further result. We prove that when the defect state has negative energy $E < 0$, under an additional assumption which we expect is generically satisfied (see (9.1) in the statement of Theorem 9.1), the truncated structure also hosts a bound state whose eigenvalue is exponentially close to E (see section 9.1). The case where $E = 0$ is not immediately amenable to our methods; see Remark 9.2 for a discussion of this.

The main ingredients of our proofs are ODE theory with periodic coefficients (Floquet theory) [27, 50] combined with a fixed point argument introduced by Dyatlov and Zworski (see section 2.8.1 of [26], where the argument is used to show that bound states of the harmonic oscillator become resonances when the potential is set to zero outside an interval). Although our proof does not generalize easily to $d > 1$ because it relies on ODE theory, we expect our result to also hold in that case and we make a general conjecture to this effect (see section 10).

1.1. Outline of paper. The outline of the paper is as follows. We will start by presenting and proving our main result in the simplest case, where the structure is symmetric under reflection about the origin (parity symmetric). We will first present our result precisely in section 2, then present the main ideas of the proof in sections 3 and 4. We provide proofs of key estimates in sections 5 and 6. We will then present our main result precisely in the case where reflection symmetry is broken in section 7, presenting the aspects of the proof which differ significantly from the reflection-symmetric case in section 8. We will finish by discussing the bound state result and conjecturing generalizations of our results in section 9.

1.2. Related work. In this section we discuss existing literature related to scattering resonances of periodic structures in one dimension. Note that we already discussed the existing literature on bound states of perturbed periodic structures in section 1.

The scattering theory of discrete and continuum periodic structures on the whole or half line perturbed by local perturbations is well studied; see, e.g., [13, 14, 15, 34, 38, 39, 44, 45]. Regarding *truncated* periodic structures, Klopp [42, 43] and Trinh [59, 60] have studied the resonances of truncated periodic structures on the whole or half-line without defects. Barra and Gaspard have studied the same problem numerically and in the limit of high energy [5]. Duchêne, Vukićević, and Weinstein [22, 23, 24, 25] and Drouot [17] have studied the scattering, homogenization, and defect modes of highly oscillatory compactly supported potentials, which are equivalent to truncated periodic structures after a rescaling. Wave packet propagation in truncated periodic structures has been studied by Molchanov and Vainberg [51, 52, 53]. Christiansen [10] has studied the resonances of “steplike” potentials which are asymptotically equal to constants with different values at large positive and negative x . Dobson et al. [16] have studied the resonances of a potential well with a thick, constant barrier in one dimension. Lin and Santosa [49] have considered the same problem in two dimensions,

when the barrier is radially symmetric.

Lin and Santosa [48] and Lin [47] have studied the resonances of one-dimensional truncated periodic Maxwell operators with defect regions. The work [48] covers the case where the structure (including the defect) has reflection symmetry about the origin, while the work [47] drops this assumption. Their results are similar to ours: they prove existence of resonances exponentially (in the truncation length) close to bound state frequencies of the untruncated periodic structures with defects. Their methods are also similar, in part: they derive algebraic resonance equations satisfied by the resonance frequency, and then prove existence of roots using a contraction mapping argument. The methods for deriving resonance equations differ between the works: in [48], this is achieved using the explicit initial conditions for the resonant state which are available when the structure is even, and in [47] this is achieved using the theory of elliptic boundary value problems. There are meaningful differences between [47, 48] and the present work, however. The first difference is that they consider a one-dimensional Maxwell system where the medium inhomogeneity enters into the equation differently from our model. However, this difference is quite minor because the two equations are equivalent under a transformation. A more significant difference is that [47, 48] assume that the periodic structure away from the defect region is *piecewise constant*, which makes the transfer/monodromy matrix for solving the Floquet ODE explicit. We make no such assumption, so our proof requires more direct ODE analysis (specifically, see sections 5 and 6). Our treatment of the case without reflection symmetry is also quite different from [47]: we generalize ODE methods to this case by solving for the initial conditions for the resonant state with the resonance frequency in the resonance equation. Finally, our results seem to give slightly sharper estimates on the distance of the resonance to the associated bound state frequency (proportional to $M^{-2}e^{-kM}$ compared to e^{-kM}).

Finally, we mention that a mathematically similar situation where bound states of a system of interacting waveguides perturb to resonances under truncation has been studied by Borisov, Exner, and Golovina [6] by different methods. Kalozoumis et al. [40] have considered a problem similar to ours and shown that the resonance of the finite structure near the bound state energy also gives rise to perfect transmission of incident plane waves at that energy, although they restrict attention to an effectively discrete model which satisfies parity symmetry.

2. Statement of main result when parity symmetry holds. We now present our main result in the simplest setting. We consider the one-dimensional continuum Schrödinger operator

$$(2.1) \quad H = D_x^2 + V(x), \quad D_x := -i\partial_x,$$

where V , the potential, is a real function. We start with the following regularity and symmetry assumptions on V .

ASSUMPTION 2.1 (regularity and translation symmetry of V). *First, we assume V is smooth: $V(x) \in C^\infty(\mathbb{R})$. Then, we assume that V can be written as*

$$(2.2) \quad V(x) = V_{\text{per}}(x) + V_{\text{def}}(x),$$

where V_{per} is periodic, i.e., $V_{\text{per}}(x+1) = V_{\text{per}}(x)$ for all $x \in \mathbb{R}$, and $V_{\text{def}}(x)$ is compactly supported, i.e., there exists $\rho \geq 0$ such that

$$(2.3) \quad |x| > \rho \implies V_{\text{def}}(x) = 0.$$

Remark 2.1. The assumption that V_{per} has periodicity 1 is made without loss of generality up to a possible rescaling of x .

Remark 2.2. The eventual periodicity assumption (2.3) is essential to our proof because it allows us to apply Floquet theory. Even so, we expect the result to still hold if this assumption is replaced by a weaker spectral gap condition; see section 10.

Now suppose that H has a bound state with positive energy, i.e., there exist $E > 0$ and $\Phi(x) \in L^2(\mathbb{R})$ such that

$$(2.4) \quad H\Phi(x) = E\Phi(x).$$

Our aim is to prove that when the structure modeled by H is truncated sufficiently far from $x = 0$, the resulting structure supports a resonance. Specifically, we aim to prove that the operator

$$(2.5) \quad H_{\text{trunc}} := D_x^2 + V_{\text{trunc}}(x),$$

where

$$(2.6) \quad V_{\text{trunc}}(x) = \begin{cases} V(x), & |x| \leq M, \\ 0, & |x| > M, \end{cases}$$

acting on $L^2(\mathbb{R})$ has a resonance $z^* \in \mathbb{C}$ with $\text{Re } z > 0$, $\text{Im } z < 0$ nearby to E in the complex plane for M sufficiently large (in particular, such that $M > \rho$).

We will present our main result first under the following simplifying symmetry assumption. We emphasize that our techniques do not fundamentally rely on this assumption, although it simplifies the statement of our result and its proof. We discuss how our result generalizes to the case where Assumption 2.2 doesn't hold in section 7.

ASSUMPTION 2.2 (parity symmetry of V). *We assume that $V(x)$ is even, i.e.,*

$$(2.7) \quad V(-x) = V(x)$$

for all $x \in \mathbb{R}$.

To present our result we require some elementary calculations and some notation. First, note that by Floquet theory (we recap the aspects of Floquet theory which are important for us in section 5), the ODE (2.4) can have at most one decaying solution for $|x| > \rho$, and hence the eigenvalue E is nondegenerate. It then follows from evenness of the potential $V(x)$ that $\Phi(x)$ is either even or odd, i.e., $\Phi(-x) = \Phi(x)$ or $\Phi(-x) = -\Phi(x)$ for all $x \in \mathbb{R}$.

When Φ is even, define $u_z(x) \in C^\infty([0, M])$ to be the solution of

$$(2.8) \quad (D_x^2 + V(x) - z)u_z = 0, \quad u_z(0) = 1, u'_z(0) = 0$$

for arbitrary $z \in \mathbb{C}$. When Φ is odd, we make the same definitions except the initial data for (2.8) should be changed to $u_z(0) = 0, u'_z(0) = 1$. Note that in either case Φ satisfies (2.8) when $z = E$. We define

$$(2.9) \quad (X_1(z), X_2(z)) := (u_z(M), u'_z(M))$$

and

$$(2.10) \quad \Theta(z) := X_2(z) - i\sqrt{z}X_1(z).$$

For the square root in (2.10), we assume $z \in \mathbb{C} \setminus (-\infty, 0]$ and choose the branch of the square root such that $\pm \operatorname{Im} z > 0 \implies \pm \operatorname{Im} \sqrt{z} > 0$. With these definitions, $z^* \in \mathbb{C}$ with $\operatorname{Re} z^* > 0$ and $\operatorname{Im} z^* < 0$ is a resonance whenever $\Theta(z^*) = 0$.

The main theorem underlying our results is the following.

THEOREM 2.1. *Let $V(x)$ satisfy Assumptions 2.1 and 2.2, and let Φ be a bound state with positive eigenvalue $E > 0$ as in (2.4). Let $\rho > 0$ be as in (2.3). Then there exist $k > 0$ and an $M_0 > \rho \geq 0$ such that for all $M \geq M_0$,*

1. $\Theta(z)$ defined by (2.10) has a unique root z^* in the ball

$$(2.11) \quad \Omega_M = \left\{ z : |z - E| \leq \frac{1}{M^2} e^{-kM} \right\}.$$

2. The location of the root z^* can be precisely characterized as

$$(2.12) \quad z^* = E - \frac{\Theta(E)}{\partial_z \Theta(E)} + O(e^{-4kM}).$$

We explain the main ideas of the proof of Theorem 2.1 in sections 3 and 4, postponing proofs of key estimates to sections 5 and 6. The overall idea of the proof is to adapt a fixed point argument introduced by Dyatlov and Zworski, who used it to prove an analogous result to Theorem 2.1 for the truncated harmonic oscillator in the semiclassical limit (see Chapter 2.8.1 of [26]). In our setting, largeness of the truncation length M can be understood as playing the role of smallness of the semiclassical parameter in Dyatlov and Zworski's proof. The most difficult step in the proof is to prove a particular map $\Psi : \mathbb{C} \rightarrow \mathbb{C}$ is a contraction in the ball Ω_M (2.11). The existence part of Theorem 2.1 (part (1)) then follows from the Banach fixed point theorem. The asymptotic formula for the resonance (part (2) of Theorem 2.1) uses the formula for the fixed point of Ψ as the limit $\lim_{n \rightarrow \infty} \Psi^n(z)$ for any $z \in \Omega$. The proof that Ψ is a contraction requires precise estimates on solutions of (2.1) which we obtain using ODE methods (specifically, Floquet theory). As a result, our proof does not generalize in a straightforward way to higher dimensions.

Remark 2.3. For $x \geq \rho$, the ODE (2.8) has periodic coefficients. Since by assumption the structure modeled by (2.8) has a bound state with energy E , Floquet theory implies the ODE must have real characteristic multipliers whose product is 1. The $k > 0$ which appears in Theorem 2.1 is simply the logarithm of the larger of these characteristic multipliers. For more details, see section 5.

The asymptotic formula for the root (2.12) is not very explicit. We can derive a more explicit formula as follows. When Φ is even, we define $v_z(x) \in C^\infty([0, M])$ to be the solution of

$$(2.13) \quad (D_x^2 + V(x) - z)v_z = 0, \quad v_z(0) = 0, v'_z(0) = 1$$

for arbitrary $z \in \mathbb{C}$. When Φ is odd, we make the same definitions except the initial data for (2.13) should be changed to $v_z(0) = -1, v'_z(0) = 0$. In either case $u_z(x)$ (2.8) and $v_z(x)$ form a fundamental solution set of the ODE (with Wronskian $u_z v'_z - u'_z v_z = 1$) appearing in (2.13). We then have the following formula for the first-order correction appearing in (2.12).

COROLLARY 2.2. *The first correction term appearing in (2.12) satisfies*

$$(2.14) \quad \frac{\Theta(E)}{\partial_z \Theta(E)} = \frac{i\sqrt{E} - [u'_E(M)v'_E(M) + Eu_E(M)v_E(M)]}{[(v'_E(M))^2 + E(v_E(M))^2] \int_0^M u_E^2(y) dy} + O(Me^{-4kM}).$$

Proof. The proof is a straightforward manipulation using the asymptotics for $\partial_z \Theta(E)$ derived in (5.15). That \sqrt{E} appears on its own comes from the fact that the Wronskian of u_E and v_E is 1. We omit the details. \square

The consequences of Theorem 2.1 and Corollary 2.2 can now be summarized as follows.

COROLLARY 2.3. *Let $V, \Phi, E > 0, \rho > 0, u_z,$ and v_z be as in Theorem 2.1 and Corollary 2.2, and let H_{trunc} be as in (2.5). Then there exist $k > 0$ and an $M_0 > \rho \geq 0$ such that for all $M \geq M_0, H_{\text{trunc}}$ has a resonance z^* such that*

$$(2.15) \quad \begin{aligned} \operatorname{Re} z^* &= E + \frac{u'_E(M)v'_E(M) + Eu_E(M)v_E(M)}{[(v'_E(M))^2 + E(v_E(M))^2] \int_0^M u_E^2(y) dy} + O(Me^{-4kM}), \\ \operatorname{Im} z^* &= \frac{-\sqrt{E}}{[(v'_E(M))^2 + E(v_E(M))^2] \int_0^M u_E^2(y) dy} + O(Me^{-4kM}). \end{aligned}$$

The associated resonant state $\Phi^*(x)$ equals

$$(2.16) \quad \Phi^*(x) = \begin{cases} u_{z^*}(x), & 0 \leq x \leq M, \\ u_{z^*}(M)e^{i\sqrt{z^*}(x-M)}, & x > M \end{cases}$$

for $x \geq 0$. When $\Phi(x)$ is even (resp., odd), $\Phi^*(x)$ is even (resp., odd).

Remark 2.4. As $M \rightarrow \infty$ the resonance pole (2.15) will converge to the defect state eigenvalue, which explains why one observes that Ω_M decreases as $M \rightarrow \infty$. In general, we suspect also that the transmission and reflection coefficients for plane wave scattering in the truncated problem converge to demonstrate the bands and the gaps of the model continuous spectrum in the infinite system (meaning the transmission coefficient should converge to 0 where there are gaps in the fully periodic model spectrum). Near energy E , the $M \rightarrow \infty$ model will have a gap, but, due to the existence of this resonance, convergence in that region may be nonuniform as observed in the related results [22, 24]. Kalozoumis et al. [40] have considered this question for an effectively discrete model with parity symmetry and found *perfect transmission* ($T = 1$) at the bound state energy. We leave further numerical study and rigorous analysis of these scattering state solutions to future works.

3. Fixed-point argument. In this section we will show how existence of a resonance nearby in the complex plane to the bound state eigenvalue E can be deduced from a fixed point argument. Recall the definitions (2.8)–(2.10) of $u_z(x)$ and $\Theta(z)$. Assuming that $\partial_z \Theta(E) \neq 0$ (we will verify this below; see (3.7)), $\Theta(z^*) = 0$ is equivalent to

$$(3.1) \quad \Psi(z^*) = z^*, \text{ where } \Psi(z) := z - \frac{\Theta(z)}{\partial_z \Theta(E)}.$$

In other words, z^* is a resonance if and only if z^* is a fixed point of the map $\Psi : \mathbb{C} \rightarrow \mathbb{C}$ defined by (3.1).

We will prove the existence of a fixed point nearby to E by showing that Ψ is a contraction in an appropriate ball centered at E for M sufficiently large. We start by defining a ball centered at E with radius $f(M)$:

$$(3.2) \quad \Omega_M := \{|z - E| \leq f(M)\}.$$

Here we assume $f(M)$ is a function such that $\lim_{M \rightarrow \infty} f(M) = 0$ but don't define its precise form yet. By the mean value theorem, Ψ is a contraction as long as $\Psi : \Omega_M \rightarrow \Omega_M$ and

$$(3.3) \quad |\partial_z \Psi(z)| \leq \frac{1}{2} \text{ for all } z \in \Omega_M.$$

Using the definition of Ψ (3.1), the condition for Ψ to be a contraction (3.3) will be satisfied if

$$(3.4) \quad |\partial_z \Theta(z) - \partial_z \Theta(E)| \leq \frac{1}{2} |\partial_z \Theta(E)| \text{ for all } z \in \Omega_M.$$

Invoking the mean value theorem again, we have that

$$(3.5) \quad |\partial_z \Theta(z) - \partial_z \Theta(E)| \leq f(M) \sup_{z \in \Omega_M} |\partial_z^2 \Theta(z)| \text{ for all } z \in \Omega_M.$$

Combining (3.5) and (3.4) establishes the following criterion for Ψ (3.1) to be a contraction in the ball Ω_M (3.2).

LEMMA 3.1. *Let u_z be as in (2.8), Θ be as in (2.10), Ψ be as in (3.1), and Ω_M be as in (3.2). Then $\Psi : \Omega_M \rightarrow \Omega_M$ is a contraction if*

$$(3.6) \quad f(M) \sup_{z \in \Omega_M} |\partial_z^2 \Theta(z)| \leq \frac{1}{2} |\partial_z \Theta(E)|.$$

We will prove the criterion (3.6) holds for sufficiently large M and $f(M) = \frac{1}{M^2} e^{-kM}$ by proving the following lemmas.

LEMMA 3.2. *There exist positive real constants C and k and $M_0 > \rho > 0$ such that for all $M \geq M_0$,*

$$(3.7) \quad |\Theta(E)| \leq C e^{-kM}, \quad |\partial_z \Theta(E)| \geq C e^{kM}.$$

Proof. The proof is given in section 5. □

LEMMA 3.3. *Let k be as in Lemma 3.2 and $f(M)$ in the definition of Ω_M be $\frac{1}{M^2} e^{-kM}$. Then there exist positive constants C and $M_0 > \rho \geq 0$ such that for all $M \geq M_0$, we have $\sup_{z \in \Omega_M} |\partial_z^2 \Theta(z)| \leq C e^{kM}$.*

Proof. The proof is given in section 6. □

We can now prove the existence part of Theorem 2.1.

Proof of part (1) of Theorem 2.1. Assuming their hypotheses, Lemmas 3.2 and 3.3 clearly imply the condition (3.6). To see that $\Psi : \Omega_M \rightarrow \Omega_M$, note that using (3.3) we have

$$(3.8) \quad |\Psi(z) - E| = |\Psi(z) - \Psi(E) + \Psi(E) - E| \leq \frac{1}{2} |z - E| + \left| \frac{\Theta(E)}{\partial_z \Theta(E)} \right|.$$

If $z \in \Omega_M$, then by definition and by Lemma 3.2 we have that $|\Psi(E) - E| \leq \frac{1}{2M^2} e^{-kM} + C e^{-2kM}$, and hence for sufficiently large M we have $\Psi(z) \in \Omega_M$. Hence by Lemma 3.1 we are done. □

The proofs of Lemmas 3.2 and 3.3 involve careful estimation of solutions of (2.8) and are the subjects of sections 5 and 6.

4. Asymptotics of the resonance. We now show how to prove the asymptotic formula part of Theorem 2.1 assuming Lemmas 3.2 and 3.3. The idea is to use the formula for the resonance in terms of iterates of the contraction Ψ :

$$(4.1) \quad z^* = \lim_{n \rightarrow \infty} \Psi^n(E),$$

although just one iterate will be enough to capture the leading-order asymptotics.

Proof of part (2) of Theorem 2.1. Let $z^{(n)} := \Psi^n(E)$. Since Ψ is a contraction we have that $|z^{(n+1)} - z^{(n)}| \leq \frac{1}{2}|z^{(n)} - z^{(n-1)}|$. By a telescoping argument it now follows that

$$(4.2) \quad |z^* - z^{(1)}| = \left| \sum_{n=1}^{\infty} z^{(n+1)} - z^{(n)} \right| \leq 2|z^{(2)} - z^{(1)}|.$$

By definition, $z^{(1)} = E - \frac{\Theta(E)}{\partial_z \Theta(E)}$ and $z^{(2)} = z^{(1)} - \frac{\Theta(z^{(1)})}{\partial_z \Theta(E)}$. Substituting these expressions into (4.2) implies

$$(4.3) \quad \left| z^* - \left(E - \frac{\Theta(E)}{\partial_z \Theta(E)} \right) \right| \leq 2 \left| \frac{\Theta \left(E - \frac{\Theta(E)}{\partial_z \Theta(E)} \right)}{\partial_z \Theta(E)} \right|.$$

The asymptotic formula (2.12) will follow immediately if we can prove that the right-hand side of (4.3) is $O(e^{-4kM})$. To this end, note that second-order Taylor expansion implies that

$$(4.4) \quad \begin{aligned} \left| \Theta \left(E - \frac{\Theta(E)}{\partial_z \Theta(E)} \right) \right| &= \left| \Theta \left(E - \frac{\Theta(E)}{\partial_z \Theta(E)} \right) - \Theta(E) + \frac{\Theta(E)}{\partial_z \Theta(E)} \partial_z \Theta(E) \right| \\ &\leq \frac{1}{2} \left| \frac{\Theta(E)}{\partial_z \Theta(E)} \right|^2 \sup_{z \in \Omega_M} |\partial_z^2 \Theta(z)|. \end{aligned}$$

Substituting (4.4) into (4.3) now gives

$$(4.5) \quad \left| z^* - \left(E - \frac{\Theta(E)}{\partial_z \Theta(E)} \right) \right| \leq \frac{1}{|\partial_z \Theta(E)|} \left| \frac{\Theta(E)}{\partial_z \Theta(E)} \right|^2 \sup_{z \in \Omega_M} |\partial_z^2 \Theta(z)|.$$

Under the hypotheses of Lemmas 3.2 and 3.3 we have that $|\partial_z \Theta(E)| \geq Ce^{kM}$, $\sup_{z \in \Omega_M} |\partial_z^2 \Theta(z)| \leq Ce^{kM}$, and $|\Theta(E)| \leq Ce^{-kM}$ for positive constants $C > 0$. The asymptotic formula (2.12) now follows immediately from substituting these estimates into (4.5). \square

5. Proof of Lemma 3.2: Bounding $\Theta(E)$ from above and $\partial_z \Theta(E)$ from below. In this section we will prove Lemma 3.2. Without loss of generality, we assume that the bound state $\Phi(x)$ is even, since the case where the bound state is odd is similar. Recall that we define $\Theta(z) = u'_z(M) - i\sqrt{z}u_z(M)$, where $u_z(x) \in C^\infty([0, M])$ is defined for any $z \in \mathbb{C}$ by

$$(5.1) \quad (D_x^2 + V(x) - z)u_z = 0, \quad u_z(0) = 1, u'_z(0) = 0.$$

Basic Floquet theory (see, e.g., [50]) implies that the ODE appearing in (5.1) has a fundamental solution set $u_{1,z}(x)$ and $u_{2,z}(x)$ which satisfy

$$(5.2) \quad u_{1,z}(x+1) = \lambda(z)u_{1,z}(x), \quad u_{2,z}(x+1) = \lambda(z)^{-1}u_{2,z}(x) \text{ for all } x \geq \rho$$

for some $\lambda(z) \in \mathbb{C}$ depending on z . For H to have a bound state with energy E , it must be that (5.1) has a decaying solution when $z = E$ and hence $|\lambda(E)| \neq 1$. Without loss of generality, we will assume $0 < \lambda(E) < 1$ so that $u_{1,E}(x)$ decays, and $u_{2,E}(x)$ grows, as $x \rightarrow \infty$. It is convenient to introduce a new constant $k > 0$ such that $\lambda(E) = e^{-k}$, so that when $z = E$, (5.2) becomes

$$(5.3) \quad u_{1,E}(x+1) = e^{-k}u_{1,E}(x), \quad u_{2,E}(x+1) = e^k u_{2,E}(x) \text{ for all } x \geq \rho.$$

Since the bound state must decay as $x \rightarrow \infty$, and (by the assumption that the bound state is even) satisfy the initial conditions (5.1), we have that (perhaps after multiplying $u_{1,E}(x)$ by a constant) $u_E(x) = u_{1,E}(x)$ for all $x \in [0, M]$. Furthermore, by letting $v_z(x)$ denote the solution of the initial value problem

$$(5.4) \quad (D_x^2 + V(x) - z)v_z = 0, \quad v_z(0) = 0, v'_z(0) = 1,$$

we must have that (perhaps after multiplying $u_{2,E}(x)$ by a constant) $v_E(x) = u_{2,E}(x)$.

We can now state two equivalent identities which are important in the coming proofs. For $\rho \leq x \leq M$, let $[x]$ be defined by the conditions

$$(5.5) \quad [x] \in [\rho, \rho + 1) \text{ and } \exists m \in \mathbb{N} \text{ such that } [x] + m = x.$$

Then (5.3) implies immediately that

$$(5.6) \quad u_E(x) = e^{-k(x-[x])}u_E([x]) \quad \text{and} \quad v_E(x) = e^{k(x-[x])}v_E([x]).$$

Equivalently, there exist 1-periodic functions $p(x), q(x) \in C^\infty([\rho, M])$ such that

$$(5.7) \quad u_E(x) = e^{-k(x-\rho)}p(x), \text{ and } v_E(x) = e^{k(x-\rho)}q(x) \text{ for all } x \geq \rho.$$

The following lemma is now clear.

LEMMA 5.1. *There exist positive constants C_1, C_2, k such that for all $M \geq \rho$, $|u_E(M)| \leq C_1 e^{-kM}$ and $|u'_E(M)| \leq C_2 e^{-kM}$.*

We can now give the proof of assertion (3.7) of Lemma 3.2.

Proof of assertion (3.7) of Lemma 3.2. The assertion follows immediately from directly bounding $\Theta(z)$ using the triangle inequality and Lemma 5.1. \square

Towards a proof of assertion on $\partial_z \Theta$ in (3.7) of Lemma 3.2, we differentiate $\Theta(z)$ with respect to z :

$$(5.8) \quad \partial_z \Theta(z) := \partial_z u'_z(M) - i\sqrt{z}\partial_z u_z(M) - i\frac{1}{2\sqrt{z}}u_z(M).$$

Differentiating (5.1) with respect to z we see that $\partial_z u_z(x)$ satisfies

$$(5.9) \quad (D_x^2 + V(x) - z)\partial_z u_z = u_z, \quad \partial_z u_z(0) = 0, \partial_z u'_z(0) = 0$$

for all $z \in \mathbb{C}$. When $z = E$, we can construct the solution of (5.9) in terms of $u_E(x)$ and $v_E(x)$ using variation of parameters. This will allow us to prove the following lemma which is the key step in bounding $\partial_z \Theta(E)$ below.

LEMMA 5.2. *Let $k > 0$ be as in Lemma 5.1. Then there exist constants $C > 0$ and $M_0 \geq \rho$ such that for all $M \geq M_0$,*

$$(5.10) \quad \left((\partial_z u'_z(M)|_{z=E})^2 + E (\partial_z u_z(M)|_{z=E})^2 \right)^{1/2} \geq C e^{kM}.$$

Proof. The proof is given in section 5.1. □

We can now prove the second assertion of Lemma 3.2.

Proof of assertion on $\partial_z \Theta$ in (3.7) of Lemma 3.2. Since every term of (5.9) is real when $z = E$, $\partial_z u_z(M)|_{z=E}$ and $\partial_z u'_z(M)|_{z=E}$ are real. It then follows that

$$(5.11) \quad |\partial_z u'_z(M) - i\sqrt{z}\partial_z u_z(M)|_{z=E} = \left((\partial_z u'_z(M)|_{z=E})^2 + E (\partial_z u_z(M)|_{z=E})^2 \right)^{1/2}.$$

Now using Lemmas 5.1 and 5.2 and the reverse triangle inequality, we can compute

$$(5.12) \quad \begin{aligned} |\partial_z \Theta(E)| &= \left| \partial_z u'_z(M) - i\sqrt{z}\partial_z u_z(M) - i\frac{1}{2\sqrt{z}}u_z(M) \right|_{z=E} \\ &\geq |\partial_z u'_z(M) - i\sqrt{z}\partial_z u_z(M)|_{z=E} + O(e^{-kM}) \geq Ce^{kM} \end{aligned}$$

for sufficiently large M . □

We now give the proof of Lemma 5.2.

5.1. Proof of Lemma 5.2. Using variation of parameters and noting that the Wronskian of u_z and v_z is 1, we have for any $z \in \mathbb{C}$ that

$$(5.13) \quad \partial_z u_z(x) = \left(\int_0^x v_z(y)u_z(y) \, dy \right) u_z(x) - \left(\int_0^x u_z^2(y) \, dy \right) v_z(x).$$

Evaluating (5.13) and its derivative with respect to x at $x = M$ and $z = E$ we have

$$(5.14) \quad \begin{aligned} \partial_z u_z(M)|_{z=E} &= \left(\int_0^M v_E(y)u_E(y) \, dy \right) u_E(M) - \left(\int_0^M u_E^2(y) \, dy \right) v_E(M), \\ \partial_z u'_z(M)|_{z=E} &= \left(\int_0^M v_E(y)u_E(y) \, dy \right) u'_E(M) - \left(\int_0^M u_E^2(y) \, dy \right) v'_E(M). \end{aligned}$$

Using (5.7) we have that $v_E(x)u_E(x)$ is 1-periodic for $x \geq \rho$. Combining this with Lemma 5.1 we have that

$$(5.15) \quad \begin{aligned} \partial_z u_z(M)|_{z=E} &= - \left(\int_0^M u_E^2(y) \, dy \right) v_E(M) + O(Me^{-kM}), \\ \partial_z u'_z(M)|_{z=E} &= - \left(\int_0^M u_E^2(y) \, dy \right) v'_E(M) + O(Me^{-kM}). \end{aligned}$$

We can now start to prove (5.10). Using (5.15) and the reverse triangle inequality, we have that

$$(5.16) \quad \begin{aligned} &\left((\partial_z u'_z(M)|_{z=E})^2 + E (\partial_z u_z(M)|_{z=E})^2 \right)^{1/2} \\ &\geq \left| \left(\left[\left(\int_0^M u_E^2(y) \, dy \right) v_E(M) \right]^2 + \left[\left(\int_0^M u_E^2(y) \, dy \right) v'_E(M) \right]^2 \right)^{1/2} - O(Me^{-kM}) \right|. \end{aligned}$$

We are done if we can show the first term inside the absolute value signs can be bounded below by Ce^{kM} where $C > 0$ is a positive constant independent of M .

We start by noting that $\int_0^M u_E^2(y) dy$ is clearly a nonzero and increasing function of M , and can hence be bounded below by a constant independent of M ; for example, $\int_0^M u_E^2(y) dy \geq \int_0^\rho u_E^2(y) dy > 0$. It follows that

$$(5.17) \quad \left(\left[\left(\int_0^M u_E^2(y) dy \right) v_E(M) \right]^2 + \left[\left(\int_0^M u_E^2(y) dy \right) v'_E(M) \right]^2 \right)^{1/2} \\ \geq \left(\int_0^\rho u_E^2(y) dy \right) \left([v_E(M)]^2 + [v'_E(M)]^2 \right)^{1/2}.$$

Using the identity (5.6) we have

$$(5.18) \quad v_E(M) = e^{k(M-[M])} v_E([M]), \text{ and } v'_E(M) = e^{k(M-[M])} v'_E([M]) \\ \implies |v_E(M)| \geq e^{kM} e^{-k(\rho+1)} \inf_{x \in [\rho, \rho+1]} |v_E(x)|, \\ \text{and } |v'_E(M)| \geq e^{kM} e^{-k(\rho+1)} \inf_{x \in [\rho, \rho+1]} |v'_E(x)|,$$

and hence (5.17) can be bounded below by

$$(5.19) \quad \geq \left(\int_0^\rho u_E^2(y) dy \right) e^{kM} e^{-k(\rho+1)} \inf_{x \in [\rho, \rho+1]} \left([v_E(x)]^2 + [v'_E(x)]^2 \right)^{1/2}.$$

We can bound $([v_E(x)]^2 + [v'_E(x)]^2)^{1/2}$ below uniformly in $x \in [\rho, \rho+1]$ using the Wronskian. For any $x \in [\rho, \rho+1]$, we have by the Cauchy–Schwarz inequality

$$(5.20) \quad 1 = |u'_E(x)v_E(x) - u_E(x)v'_E(x)| \leq ([u_E(x)]^2 + [u'_E(x)]^2)^{1/2} ([v_E(x)]^2 + [v'_E(x)]^2)^{1/2},$$

and hence

$$(5.21) \quad ([v_E(x)]^2 + [v'_E(x)]^2)^{1/2} \geq \frac{1}{\sup_{x \in [\rho, \rho+1]} ([u_E(x)]^2 + [u'_E(x)]^2)^{1/2}}.$$

Combining (5.21) with (5.19) and substituting into (5.16), we are done.

6. Proof of Lemma 3.3: Bounding $\partial_z^2 \Theta(z)$ uniformly for $z \in \Omega_M$. We now seek to bound $\partial_z^2 \Theta(z)$ uniformly in z in a ball centered at E . Differentiating $\Theta(z)$ gives

$$(6.1) \quad \partial_z^2 \Theta(z) = \partial_z^2 u'_z(M) + \frac{1}{4} i z^{-3/2} u_z(M) - i z^{-1/2} \partial_z u_z(M) - i z^{1/2} \partial_z^2 u_z(M),$$

and hence we are done if we can bound $\partial_z^2 u'_z(M)$, $u_z(M)$, $\partial_z u_z(M)$, and $\partial_z^2 u_z(M)$ uniformly in z for z nearby to E .

By differentiating the initial value problem (2.8) we have that $\partial_z^2 u_z$ satisfies

$$(6.2) \quad (D_x^2 + V(x) - z) \partial_z^2 u_z = 2 \partial_z u_z, \quad \partial_z^2 u(0) = \partial_z^2 u'(0) = 0,$$

while $\partial_z u_z$ and u_z satisfy

$$(6.3) \quad (D_x^2 + V(x) - z) \partial_z u_z = u_z, \quad \partial_z u_z(0) = 0, \partial_z u'_z(0) = 0,$$

$$(6.4) \quad (D_x^2 + V(x) - z) u_z = 0, \quad u_z(0) = 1, u'_z(0) = 0,$$

respectively. The key step in the proof of Lemma 3.2 is the following.

LEMMA 6.1. *Let $x > 0$ be arbitrary, and let $z \in \mathbb{C}$ be such that $|z - E| \leq \frac{1}{2xC^*(e^{kx}+1)}$. Then there exists a positive constant $C^* > 0$ such that the following estimates hold:*

$$(6.5) \quad \max \{|u_z(x)|, |u'_z(x)|\} \leq 2C^*(e^{kx} + 1),$$

$$(6.6) \quad \max \{|\partial_z u_z(x)|, |\partial_z u'_z(x)|\} \leq 4C^*(e^{kx} + 1),$$

$$(6.7) \quad \max \{|\partial_z^2 u_z(x)|, |\partial_z^2 u'_z(x)|\} \leq 8C^*(e^{kx} + 1).$$

Proof. The proofs of (6.5) and (6.6) are given in sections 6.1 and 6.2. Since the proof of (6.7) is so similar to that of (6.6), we omit it. \square

We can now give the proof of Lemma 3.3.

Proof of Lemma 3.3. If $f(M) = \frac{1}{M^2}e^{-kM}$, then there exists a $M_0 > 0$ such that for all $M \geq M_0$, $z \in \Omega_M$ implies that $|z - E| \leq \frac{1}{2MC^*(e^{kM}+1)}$. Applying Lemma 6.1 to (6.1) and using the triangle inequality yields

$$\begin{aligned} |\partial_z \Theta(z)| &\leq 8C^*(e^{kM} + 1) + \frac{1}{4}|z|^{-3/2}2C^*(e^{kM} + 1) \\ &\quad + |z|^{-1/2}4C^*(e^{kM} + 1) + |z|^{1/2}8C^*(e^{kM} + 1). \end{aligned}$$

To bound the terms involving z we note that $|z|^{1/2} = |z - E + E|^{1/2} \leq |E|^{1/2} + C|z - E|$, where $C = \sup_{z \in \Omega_M} \frac{d}{dz}|z|^{1/2}$. Since we assume $E > 0$, we then have that (perhaps after taking M_0 larger) $|\partial_z \Theta(z)| \leq Ce^{kM}$ for some constant $C > 0$. \square

6.1. Proof of assertion (6.5) of Lemma 6.1: Bounding solutions of (6.4) uniformly for $z \in \Omega_M$. The idea is to use Picard iteration to solve (6.4) perturbatively about $z = E$. We start by writing (6.4) as

$$(6.8) \quad (D_x^2 + V(x) - E)u_z = (z - E)u_z, \quad u_z(0) = 1, u'_z(0) = 0,$$

and then as a first-order system for $\mathbf{u}_z := (u_z(x), u'_z(x))^T$:

$$(6.9) \quad \mathbf{u}'_z = H(x)\mathbf{u}_z + \tilde{H}\mathbf{u}_z, \quad \mathbf{u}_z(0) = (1, 0)^T,$$

where

$$(6.10) \quad H(x) := \begin{pmatrix} 0 & 1 \\ V(x) - E & 0 \end{pmatrix}, \quad \tilde{H} := \begin{pmatrix} 0 & 0 \\ E - z & 0 \end{pmatrix}.$$

Note that $H(x + 1) = H(x)$ for $x \geq \rho$.

When $z = E$ so that $\tilde{H} = 0$, (6.9) has the solution $\mathbf{u}_z(x) = U_E(x)\mathbf{u}_z(0)$, where $U_E(x)$ is the solution operator

$$(6.11) \quad U_E(x) := \begin{pmatrix} u_E(x) & v_E(x) \\ u'_E(x) & v'_E(x) \end{pmatrix}.$$

Recalling (5.7), we have that

$$(6.12) \quad u_E(x) = e^{-k(x-\rho)}p(x), \quad u'_E(x) = e^{-k(x-\rho)}(-kp(x) + p'(x)),$$

where $p(x) \in C^\infty(\mathbb{R})$ is 1-periodic, and $k > 0$, for all $x \geq \rho$. Similarly, we have that

$$(6.13) \quad v_E(x) = e^{k(x-\rho)}q(x), \quad v'_E(x) = e^{k(x-\rho)}(kq(x) + q'(x)),$$

where $q(x)$ is 1-periodic, and $k > 0$, for all $x \geq \rho$. It is now trivial to prove pointwise bounds on each of the entries of $U_E(x)$; for example,

$$(6.14) \quad |v_E(x)| \leq \sup_{0 \leq x \leq \rho} |v_E(x)| + e^{k(x-\rho)} \sup_{\rho \leq x \leq \rho+1} |q(x)|.$$

From these pointwise bounds it is clear that there exists a constant $C^* > 0$ such that

$$(6.15) \quad \begin{aligned} \|U_E(x)\mathbf{f}\|_\infty &= \sup \{|u_E(x)f_1 + v_E(x)f_2|, |u'_E(x)f_1 + v'_E(x)f_2|\} \\ &\leq 2 \sup \{|u_E(x)|, |v_E(x)|, |u'_E(x)|, |v'_E(x)|\} \|\mathbf{f}\|_\infty \leq C^* (e^{kx} + 1) \|\mathbf{f}\|_\infty. \end{aligned}$$

We now seek to solve (6.9) for $|z - E|$ small by Picard iteration. Using Duhamel's formula, we can rewrite (6.9) as the fixed point equation

$$(6.16) \quad \mathbf{u}_z(x) = U_E(x)\mathbf{u}_z(0) + \int_0^x U_E(x-y)\tilde{H}\mathbf{u}_z(y) dy.$$

For any $X \geq 0$, we define an operator

$$(6.17) \quad T_X : \mathbf{f}(x) \mapsto U(x)\mathbf{f}(0) + \int_0^x U(x-y)\tilde{H}\mathbf{f}(y) dy$$

acting on the Banach space $B_X := \{\mathbf{f} \in C([0, X]; \mathbb{C}^2) : \mathbf{f}(0) = \mathbf{u}_z(0)\}$, equipped with the sup norm. To see when this operator is a contraction we consider

$$(6.18) \quad \|T_X\mathbf{f}(x) - T_X\mathbf{g}(x)\|_\infty = \left\| \int_0^x U(x-y)\tilde{H}(\mathbf{f}(y) - \mathbf{g}(y)) dy \right\|_\infty.$$

Since $\|\tilde{H}\|_\infty$ is clearly bounded by $|z - E|$, we have

$$(6.19) \quad \begin{aligned} \|T_X\mathbf{f}(x) - T_X\mathbf{g}(x)\|_\infty &= \left\| \int_0^x U(x-y)\tilde{H}(\mathbf{f}(y) - \mathbf{g}(y)) dy \right\|_\infty \\ &\leq X \sup_{0 \leq x \leq X} \|U(x)\|_\infty |z - E| \|\mathbf{f}(y) - \mathbf{g}(y)\|_\infty \\ &\leq C^* X (e^{kX} + 1) |z - E| \|\mathbf{f}(x) - \mathbf{g}(x)\|_\infty. \end{aligned}$$

It follows that T_X is a contraction as long as $|z - E| < \frac{1}{C^* X (e^{kX} + 1)}$. In this case we have the following formula for $\mathbf{u}_z(x)$:

$$(6.20) \quad \mathbf{u}_z(x) = \lim_{n \rightarrow \infty} T^n \mathbf{u}_{z,0},$$

where $\mathbf{u}_{z,0}$ denotes the function equal to the constant $\mathbf{u}_z(0)$ on the interval $[0, X]$. Equation (6.20) written out is

$$(6.21) \quad \begin{aligned} \mathbf{u}_z(x) &= U_E(x)\mathbf{u}_z(0) + \int_0^x U_E(x-y)\tilde{H}U_E(y)\mathbf{u}_z(0) dy \\ &+ \int_0^x U_E(x-y)\tilde{H} \int_0^y U_E(y-y_1)\tilde{H}U_E(y_1)\mathbf{u}_z(0) dy_1 dy + \dots \end{aligned}$$

The second term on the right-hand side can be bounded as

$$(6.22) \quad \begin{aligned} \left| \int_0^x U_E(x-y)\tilde{H}U_E(y)\mathbf{u}_z(0) dy \right| &\leq x \sup_{0 \leq y \leq x} |U_E(x-y)\tilde{H}U_E(y)\mathbf{u}_z(0)| \\ &\leq x C^* (e^{kx} + 1) |z - E| C^* (e^{kx} + 1) \\ &= x |z - E| (C^* (e^{kx} + 1))^2. \end{aligned}$$

Bounding the other terms on the right-hand side similarly, we have

$$(6.23) \quad \begin{aligned} |\mathbf{u}_z(x)| &\leq C^*(e^{kx} + 1) + x|z - E|(C^*(e^{kx} + 1))^2 + x^2|z - E|^2(C^*(e^{kx} + 1))^3 + \dots \\ &= C^*(e^{kx} + 1) (1 + x|z - E|(C^*(e^{kx} + 1)) + x^2|z - E|^2(C^*(e^{kx} + 1))^2 + \dots). \end{aligned}$$

Hence, whenever $x|z - E|C^*(e^{kx} + 1) < 1$, we have that

$$(6.24) \quad |\mathbf{u}_z(x)| \leq \frac{C^*(e^{kx} + 1)}{1 - x|z - E|C^*(e^{kx} + 1)}.$$

By taking $|z - E| \leq \frac{1}{2xC^*(e^{kx+1})}$ we have the desired bound (6.5).

6.2. Proof of assertion (6.6) of Lemma 6.1: Bounding solutions of (6.3) uniformly for $z \in \Omega_M$. We start by rewriting (6.3) as

$$(6.25) \quad (D_x^2 + V(x) - E)\partial_z u_z = (z - E)\partial_z u_z + u_z, \quad \partial_z u_z(0) = 0, \partial_z u'_z(0) = 0.$$

We can write (6.25) as a first-order system just as in (6.9). Using Duhamel’s formula and the fact that $\partial_z \mathbf{u}_z(0) = 0$, we have that

$$(6.26) \quad \partial_z \mathbf{u}_z(x) = \int_0^x U(x - y) [\tilde{H}\partial_z \mathbf{u}_z(y) + \mathbf{u}_z(y)] dy,$$

where \tilde{H} is as in (6.10). The map $T'_X : \mathbf{f}(x) \mapsto \int_0^x U_E(x - y) [\tilde{H}\mathbf{f}(y) + \mathbf{u}_z(y)] dy$ is clearly a contraction on the Banach space of functions on $[0, X]$ with $\mathbf{f}(0) = 0$ equipped with the sup norm under the same conditions as before, i.e., as long as $XC^*(e^{kX} + 1)|z - E| < 1$. Starting the iteration with the constant zero function, we have the analogous representation as (6.21) for the solution of (6.25):

$$(6.27) \quad \partial_z \mathbf{u}_z(x) = \int_0^x U_E(x - y)\mathbf{u}_z(y) dy + \int_0^x U_E(x - y)\tilde{H} \int_0^y U_E(y - y_1)\mathbf{u}_z(y_1) dy_1 dy + \dots$$

Replacing $\mathbf{u}_z(y)$ everywhere by its expansion (6.21), we have for the first term on the right-hand side in (6.27) that

$$(6.28) \quad \begin{aligned} &\int_0^x U_E(x - y)\mathbf{u}_z(y) dy \\ &= \int_0^x U_E(x)\mathbf{u}_z(0) dy + \int_0^x U_E(x - y) \int_0^y U_E(y - y_1)\tilde{H}U_E(y_1)\mathbf{u}_z(0) dy_1 dy + \dots, \end{aligned}$$

and hence

$$(6.29) \quad \begin{aligned} \int_0^x U_E(x - y)\mathbf{u}_z(y) dy &\leq xC^*(e^{kx} + 1) + x^2 (C^*(e^{kx} + 1))^2 |z - E| + \dots \\ &\leq 2xC^*(e^{kx} + 1) \end{aligned}$$

whenever $xC^*(e^{kx} + 1)|z - E| \leq \frac{1}{2}$. As for the second term in (6.27), we have

$$(6.30) \quad \begin{aligned} &\int_0^x U_E(x - y)\tilde{H} \int_0^y U_E(y - y_1)\mathbf{u}_z(y_1) dy_1 dy = \int_0^x U_E(x - y)\tilde{H} \int_0^y U_E(y)\mathbf{u}_z(0) dy_1 dy \\ &+ \int_0^x U_E(x - y)\tilde{H} \int_0^y U_E(y - y_1) \int_0^{y_1} U_E(y_1 - y_2)\tilde{H}U_E(y_2)\mathbf{u}_z(0) dy_2 dy_1 dy + \dots, \end{aligned}$$

and hence

$$(6.31) \quad \begin{aligned} & \left| \int_0^x U_E(x-y) \tilde{H} \int_0^y U_E(y-y_1) \mathbf{u}_z(y_1) dy_1 dy \right| \\ & \leq x^2 (C^*(e^{kx} + 1))^2 |z - E| + x^3 (C^*(e^{kx} + 1))^3 |z - E|^2 + \dots \\ & \leq 2x^2 (C^*(e^{kx} + 1))^2 |z - E| \end{aligned}$$

whenever $x C^*(e^{kx} + 1) |z - E| < \frac{1}{2}$. Bounding successive terms of (6.27) similarly, we have that

$$(6.32) \quad \begin{aligned} & |\partial_z \mathbf{u}_z(x)| \\ & \leq 2x C^*(e^{kx} + 1) + 2x^2 (C^*(e^{kx} + 1))^2 |z - E| + 2x^3 (C^*(e^{kx} + 1))^3 |z - E|^2 + \dots \\ & \leq 4x C^*(e^{kx} + 1) \end{aligned}$$

whenever $x C^*(e^{kx} + 1) |z - E| < \frac{1}{2}$, as desired.

7. Generalization of our main result when parity symmetry does not necessarily hold. In this section we present a generalization of the result presented in section 2 which covers the case where the parity symmetry assumption (Assumption 2.2) does not hold. Although many of the ideas presented in the previous sections, particularly the use of Floquet theory, carry over to this setting, there are significant differences between the results and proofs. We review the parts of the proof which are significantly different in this case in section 8.

We again consider the one-dimensional Schrödinger operator (2.1), assuming the potential V is smooth and 1-periodic outside the interval $[-\rho, \rho]$ for some $\rho > 0$ (Assumption 2.1). We again assume the existence of a bound state $\Phi(x)$ with positive eigenvalue $E > 0$ (2.4). When $\Phi(0) \neq 0$ (note that after multiplying by a constant we can assume $\Phi(0) = 1$), define $u_\zeta(x) \in C^\infty([-M, M])$ and $v_\zeta(x) \in C^\infty([-M, M])$ as the solutions of

$$(7.1) \quad \begin{aligned} (D_x^2 + V(x) - z)u_\zeta &= 0, & u_\zeta(0) &= 1, u'_\zeta(0) = w, \\ (D_x^2 + V(x) - z)v_\zeta &= 0, & v_\zeta(0) &= \frac{-w}{1+w^2}, v'_\zeta(0) = \frac{1}{1+w^2} \end{aligned}$$

for arbitrary $\zeta = (w, z) \in \mathbb{C}^2$, and let $\eta = (\Phi'(0), E)$. Note that with these definitions u_ζ and v_ζ form a fundamental solution set whose Wronskian is 1 and $u_\eta(x) = \Phi(x)$ for $|x| \leq M$. When $\Phi(0) = 0$ (note that after multiplying by a constant we can assume $\Phi'(0) = 1$), define $u_\zeta(x)$ and $v_\zeta(x)$ by

$$(7.2) \quad \begin{aligned} (D_x^2 + V(x) - z)u_\zeta &= 0, & u_\zeta(0) &= -w, u'_\zeta(0) = 1, \\ (D_x^2 + V(x) - z)v_\zeta &= 0, & v_\zeta(0) &= \frac{-1}{1+w^2}, v'_\zeta(0) = \frac{-w}{1+w^2}, \end{aligned}$$

and let $\eta = (0, E)$ (see Remark 8.1 for an explanation of the convention we choose in (7.2)). Again, u_ζ and v_ζ form a fundamental solution set and $u_\eta(x) = \Phi(x)$ for $|x| \leq M$. Since $\Phi(x)$ is a bound state, via Floquet theory we have that u_η must exponentially decay and v_η must exponentially grow. We define

$$(7.3) \quad (X_1^\pm(\zeta), X_2^\pm(\zeta)) := (u_\zeta(\pm M), u'_\zeta(\pm M)),$$

and let

$$(7.4) \quad \Theta^\pm(\zeta) := X_2^\pm(\zeta) \mp i\sqrt{z}X_1^\pm(\zeta).$$

With the same conventions on the square root as in the case where parity symmetry holds (see below (2.10)), we have that when $E > 0$, z^* is a resonance of H_{trunc} if and only if

$$(7.5) \quad \Theta(\zeta^*) = 0, \quad \text{where } \Theta(\zeta) := \begin{pmatrix} \Theta^+(\zeta) \\ \Theta^-(\zeta) \end{pmatrix},$$

where $\zeta^* = (w^*, z^*)$ for some $w^* \in \mathbb{C}$.

In this setting, the counterpart of Theorem 2.1 is as follows.

THEOREM 7.1. *Let $V(x)$ satisfy Assumption 2.1, let $\rho > 0$ be as in (2.3), and let Φ be a bound state with eigenvalue $E > 0$ as in (2.4). Then there exist $k > 0$ and an $M_0 > \rho \geq 0$ such that for all $M \geq M_0$,*

1. $\Theta(\zeta)$ in (7.5) has a unique root ζ^* in the ball $\Omega_M = \{\zeta : |\zeta - \eta| \leq \frac{1}{M^2}e^{-kM}\}$.
2. The location of the root ζ^* can be precisely characterized as

$$(7.6) \quad \zeta^* = \eta - \Xi\Theta(\eta) + O(e^{-4kM}),$$

where Ξ is the matrix

$$(7.7) \quad \Xi := \frac{1}{\mathcal{N}(\eta)} \begin{pmatrix} \partial_z \Theta^-(\eta) & -\partial_z \Theta^+(\eta) \\ -\partial_w \Theta^-(\eta) & \partial_w \Theta^+(\eta) \end{pmatrix},$$

$$\text{and } \mathcal{N}(\eta) := \partial_w \Theta^+(\eta) \partial_z \Theta^-(\eta) - \partial_z \Theta^+(\eta) \partial_w \Theta^-(\eta).$$

The overall idea of the proof of Theorem 7.1 is the same as that of Theorem 2.1. We give a sketch of the proof here, postponing a discussion of the details which differ from the proof of Theorem 2.1 to section 8. Define $\Psi : \mathbb{C}^2 \rightarrow \mathbb{C}^2$ by

$$(7.8) \quad \Psi(\zeta) := \zeta - \Xi\Theta(\zeta),$$

where Ξ is defined by (7.7). Assuming $\mathcal{N}(\eta) \neq 0$, then $\det \Xi = \frac{1}{[\mathcal{N}(\eta)]^3}$ so that Ξ is invertible, and hence $\Psi(\zeta) = \zeta \iff \Theta(\zeta) = 0$. It remains to show that Ψ is a contraction in the ball

$$(7.9) \quad \Omega_M := \left\{ \zeta \in \mathbb{C}^2 : |\zeta - \eta| < \frac{1}{M^2}e^{-kM} \right\},$$

where k characterizes the exponential decay of the bound state just as in the proof of Theorem 2.1 (recall section 5). Parts (1) and (2) of the theorem then follow from the Banach fixed point theorem and the asymptotic formula for the fixed point as $\lim_{n \rightarrow \infty} \Psi^n(\eta)$, respectively. For the proofs that $\mathcal{N}(\eta) \neq 0$ and that Ψ defined by (7.8) with Ξ as in (7.7) is a contraction in Ω_M , see section 8.

Remark 7.1. The matrix Ξ is the inverse of

$$\begin{pmatrix} \partial_w \Theta^+(\eta) & \partial_z \Theta^+(\eta) \\ \partial_w \Theta^-(\eta) & \partial_z \Theta^-(\eta) \end{pmatrix},$$

which is the Jacobian of the map $\zeta \mapsto (\Theta^+(\zeta), \Theta^-(\zeta))$ evaluated at $\zeta = \eta$. This is consistent with the parity symmetry case (compare (7.6) with (2.12)), where $\frac{1}{\partial_z \Theta(E)}$ is the inverse of $\partial_z \Theta(E)$, which is the Jacobian of the map $z \mapsto \Theta(z)$ evaluated at $z = E$.

Remark 7.2. It is straightforward to derive analogues of Corollaries 2.2 and 2.3 in this context, and check that, in the special case where parity symmetry holds, these expressions reduce to the results of those corollaries as expected. Since the expressions are more complex in this case, we omit these analogues.

Remark 7.3. We remark on further generalizations of our result which should follow from an essentially identical analysis. First, recall that we assume the structure is truncated at $x = \pm M$ (2.6). Our result could be generalized to the case where the structure is truncated at some $M_+ > 0$ and $M_- < 0$ where $M_+ \neq -M_-$ in the limit where $M_{\pm} \rightarrow \pm\infty$. Second, our result should even generalize to the case of differing periodic structures either side of the defect region, even with differing periods. Since extending our results to these settings would complicate the statement of our results and would not require substantial modifications of the proof, we do not consider these cases here.

8. Proof of Theorem 7.1: Derivation of Ξ and proof of $\mathcal{N}(\boldsymbol{\eta}) \neq 0$. In this section we present the parts of the proof of Theorem 7.1 which differ substantially from the proof of Theorem 2.1. Specifically, we show that the form of Ξ (7.7) makes the map Ψ (7.8) a contraction in the ball Ω_M (7.9), and prove that $\mathcal{N}(\boldsymbol{\eta}) \neq 0$ so that Ξ is well defined.

We will first show that the form of Ξ (7.7) makes Ψ a contraction in the ball Ω_M . Writing $\Psi(\boldsymbol{\zeta}) = (\Psi_1(\boldsymbol{\zeta}), \Psi_2(\boldsymbol{\zeta}))^\top$, by Taylor's theorem we have that Ψ is a contraction if every element of the Jacobian matrix

$$(8.1) \quad J := \begin{pmatrix} \partial_w \Psi_1 & \partial_z \Psi_1 \\ \partial_w \Psi_2 & \partial_z \Psi_2 \end{pmatrix}$$

can be bounded uniformly by $\frac{1}{2}$ in Ω_M . Recalling the form of Ψ (7.8), writing

$$\Xi = \begin{pmatrix} \Xi_{11} & \Xi_{12} \\ \Xi_{21} & \Xi_{22} \end{pmatrix},$$

and assuming Ξ is independent of $\boldsymbol{\zeta}$, we have that

$$(8.2) \quad J = \begin{pmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{pmatrix} = \begin{pmatrix} 1 - \Xi_{11}\partial_w\Theta^+ - \Xi_{12}\partial_w\Theta^- & -\Xi_{11}\partial_z\Theta^+ - \Xi_{12}\partial_z\Theta^- \\ -\Xi_{21}\partial_w\Theta^+ - \Xi_{22}\partial_w\Theta^- & 1 - \Xi_{21}\partial_z\Theta^+ - \Xi_{22}\partial_z\Theta^- \end{pmatrix}.$$

Substituting the form of Ξ given in (7.7) (we will prove in Lemma 8.1 that $\mathcal{N}(\boldsymbol{\eta}) \neq 0$ so that Ξ is well defined), the diagonal entries of J are

$$(8.3) \quad \begin{aligned} J_{11} &= 1 - \frac{\partial_w\Theta^+(\boldsymbol{\zeta})\partial_z\Theta^-(\boldsymbol{\eta}) - \partial_z\Theta^+(\boldsymbol{\eta})\partial_w\Theta^-(\boldsymbol{\zeta})}{\mathcal{N}(\boldsymbol{\eta})}, \\ J_{22} &= 1 - \frac{\partial_w\Theta^+(\boldsymbol{\eta})\partial_z\Theta^-(\boldsymbol{\zeta}) - \partial_z\Theta^+(\boldsymbol{\zeta})\partial_w\Theta^-(\boldsymbol{\eta})}{\mathcal{N}(\boldsymbol{\eta})}, \end{aligned}$$

while the off-diagonal terms are

$$(8.4) \quad \begin{aligned} J_{12} &= -\frac{\partial_z\Theta^+(\boldsymbol{\zeta})\partial_z\Theta^-(\boldsymbol{\eta}) - \partial_z\Theta^+(\boldsymbol{\eta})\partial_z\Theta^-(\boldsymbol{\zeta})}{\mathcal{N}(\boldsymbol{\eta})}, \\ J_{21} &= -\frac{\partial_w\Theta^+(\boldsymbol{\zeta})\partial_w\Theta^-(\boldsymbol{\eta}) - \partial_w\Theta^+(\boldsymbol{\eta})\partial_w\Theta^-(\boldsymbol{\zeta})}{\mathcal{N}(\boldsymbol{\eta})}. \end{aligned}$$

To see that this choice of Ξ makes the entries of J small for $z \in \Omega_M$ and M sufficiently large, note that we can rewrite the entries of J as

$$\begin{aligned}
 (8.5) \quad J_{11} &= \frac{1}{\mathcal{N}(\boldsymbol{\eta})} [(\partial_w \Theta^+(\boldsymbol{\eta}) - \partial_w \Theta^+(\boldsymbol{\zeta})) \partial_z \Theta^-(\boldsymbol{\eta}) - \partial_z \Theta^+(\boldsymbol{\eta}) (\partial_w \Theta^-(\boldsymbol{\eta}) - \partial_w \Theta^-(\boldsymbol{\zeta}))], \\
 J_{22} &= \frac{1}{\mathcal{N}(\boldsymbol{\eta})} [\partial_w \Theta^+(\boldsymbol{\eta}) (\partial_z \Theta^-(\boldsymbol{\eta}) - \partial_z \Theta^-(\boldsymbol{\zeta})) - (\partial_z \Theta^+(\boldsymbol{\eta}) - \partial_z \Theta^+(\boldsymbol{\zeta})) \partial_w \Theta^-(\boldsymbol{\eta})], \\
 J_{12} &= \frac{1}{\mathcal{N}(\boldsymbol{\eta})} [\partial_z \Theta^+(\boldsymbol{\eta}) (\partial_z \Theta^-(\boldsymbol{\zeta}) - \partial_z \Theta^-(\boldsymbol{\eta})) + (\partial_z \Theta^+(\boldsymbol{\eta}) - \partial_z \Theta^+(\boldsymbol{\zeta})) \partial_z \Theta^-(\boldsymbol{\eta})], \\
 J_{21} &= \frac{1}{\mathcal{N}(\boldsymbol{\eta})} [\partial_w \Theta^+(\boldsymbol{\eta}) (\partial_w \Theta^-(\boldsymbol{\zeta}) - \partial_w \Theta^-(\boldsymbol{\eta})) - (\partial_w \Theta^+(\boldsymbol{\zeta}) - \partial_w \Theta^+(\boldsymbol{\eta})) \partial_w \Theta^-(\boldsymbol{\eta})].
 \end{aligned}$$

We see that every component of J is a sum of two terms. We will show that each component can be bounded by $\frac{1}{2}$ by showing that each of these terms can be bounded by $\frac{1}{4}$. The proofs follow logic similar to that given in section 3. To give the idea, we first consider a representative term before making the necessary estimates precise. We aim to prove that, for example,

$$(8.6) \quad \left| \frac{1}{\mathcal{N}(\boldsymbol{\eta})} (\partial_z \Theta^+(\boldsymbol{\eta}) - \partial_z \Theta^+(\boldsymbol{\zeta})) \partial_w \Theta^-(\boldsymbol{\eta}) \right| < \frac{1}{4},$$

or equivalently, $|\partial_z \Theta^+(\boldsymbol{\eta}) - \partial_z \Theta^+(\boldsymbol{\zeta})| |\partial_w \Theta^-(\boldsymbol{\eta})| < \frac{1}{4} |\mathcal{N}(\boldsymbol{\eta})|$ for all $z \in \Omega_M$. By the mean value theorem, we have that

$$(8.7) \quad |\partial_z \Theta^+(\boldsymbol{\eta}) - \partial_z \Theta^+(\boldsymbol{\zeta})| \leq |\boldsymbol{\zeta} - \boldsymbol{\eta}| \sup_{z \in \Omega_M} |\partial_z^2 \Theta^+(\boldsymbol{\zeta})|$$

for $\boldsymbol{\zeta} \in \Omega_M$. Since for $\boldsymbol{\zeta} \in \Omega_M$, $|\boldsymbol{\zeta} - \boldsymbol{\eta}|$ is exponentially small in M , estimate (8.6) is proved if we can show that

$$(8.8) \quad \sup_{z \in \Omega_M} |\partial_z^2 \Theta^+(\boldsymbol{\zeta})| \leq C e^{kM}, \quad |\partial_w \Theta^-(\boldsymbol{\eta})| \leq C e^{kM}, \quad \text{and} \quad |\mathcal{N}(\boldsymbol{\eta})| \geq C e^{2kM}$$

for constants $k > 0$ and $C > 0$. It is clear that with analogous bounds as in (8.8), the other terms appearing in (8.5) can be bounded along the same lines.

Now that the basic idea has been established, we make precise the lemmas which are necessary to prove that Ψ is a contraction. First, we require a lemma analogous to Lemma 3.2.

LEMMA 8.1. *Let $\Theta^\pm(\boldsymbol{\zeta})$ be as in (7.4). There exist positive constants C and k and $M_0 > \rho > 0$ such that for all $M \geq M_0$,*

$$(8.9) \quad \mathcal{N}(\boldsymbol{\eta}) := \partial_w \Theta^+(\boldsymbol{\eta}) \partial_z \Theta^-(\boldsymbol{\eta}) - \partial_z \Theta^+(\boldsymbol{\eta}) \partial_w \Theta^-(\boldsymbol{\eta})$$

satisfies $|\mathcal{N}(\boldsymbol{\eta})| \geq C e^{2kM}$.

Second, we require a lemma analogous to Lemma 3.3.

LEMMA 8.2. *Let k be as in Lemma 8.1 and Ω_M be as in (7.9). Then there exist positive constants C and $M_0 > \rho > 0$ such that for all $M \geq M_0$ the following estimates hold:*

$$(8.10) \quad |\partial_z \Theta^\pm(\boldsymbol{\eta})| \leq C e^{kM}, \quad |\partial_w \Theta^\pm(\boldsymbol{\eta})| \leq C e^{kM},$$

$$(8.11) \quad \sup_{\boldsymbol{\zeta} \in \Omega_M} |\partial_z^2 \Theta^\pm(\boldsymbol{\zeta})| \leq C e^{kM}, \quad \sup_{\boldsymbol{\zeta} \in \Omega_M} |\partial_w^2 \Theta^\pm(\boldsymbol{\zeta})| \leq C e^{kM}.$$

We explain the important points of these proofs, particularly those points which differ from the proofs of Lemmas 3.2 and 3.3, in the following section.

8.1. Proofs of Lemmas 8.1 and 8.2. Using the definitions of $\Theta^\pm(\boldsymbol{\eta})$ (7.3)–(7.4) we have that

$$(8.12) \quad \begin{aligned} \partial_z \Theta^\pm(\boldsymbol{\zeta}) &= \partial_z u'_\zeta(\pm M)|_{\zeta=\boldsymbol{\eta}} \mp i\sqrt{E} \partial_z u_\zeta(\pm M)|_{\zeta=\boldsymbol{\eta}} \mp i \frac{1}{2\sqrt{E}} u_\zeta(\pm M)|_{\zeta=\boldsymbol{\eta}}, \\ \partial_w \Theta^\pm(\boldsymbol{\zeta}) &= \partial_w u'_\zeta(\pm M)|_{\zeta=\boldsymbol{\eta}} \mp i\sqrt{E} \partial_w u_\zeta(\pm M)|_{\zeta=\boldsymbol{\eta}}. \end{aligned}$$

Suppose that $\Phi(0) \neq 0$ so that u_ζ and v_ζ are defined by (7.1). Differentiating the equation for u_ζ we have that $\partial_w u_\zeta(x)$ satisfies

$$(8.13) \quad (D_x^2 + V(x) - z) \partial_w u_\zeta = 0, \quad \partial_w u_\zeta(0) = 0, \quad \partial_w u'_\zeta(0) = 1,$$

which has the unique solution

$$(8.14) \quad \partial_w u_\zeta(x) = \frac{w}{1+w^2} u_\zeta(x) + v_\zeta(x).$$

If instead $\Phi(0) = 0$, so that u_ζ and v_ζ are defined by (7.2), then $\partial_w u_\zeta(x)$ satisfies

$$(8.15) \quad (D_x^2 + V(x) - z) \partial_w u_\zeta = 0, \quad \partial_w u_\zeta(0) = 1, \quad \partial_w u'_\zeta(0) = 0,$$

which has the unique solution

$$(8.16) \quad \partial_w u_\zeta(x) = \frac{w}{1+w^2} u_\zeta(x) + v_\zeta(x).$$

Remark 8.1. Note that by virtue of the convention we chose for u_ζ and v_ζ in (7.2), the formulas for $\partial_w u_\zeta$ in (8.14) and (8.16) match. This allows us to write formulas which are valid in both cases without modification.

By variation of parameters as in section 5.1 we have that

$$(8.17) \quad \partial_z u_\zeta(x) = \left(\int_0^x v_\zeta(y) u_\zeta(y) dy \right) u_\zeta(x) - \left(\int_0^x u_\zeta^2(y) dy \right) v_\zeta(x).$$

We now argue as in section 5. Setting $\boldsymbol{\zeta} = \boldsymbol{\eta}$, by Floquet theory and the assumption that $u_\boldsymbol{\eta}(x) = \Phi(x)$ for $|x| \leq M$, we have that $u_\boldsymbol{\eta}(x)$ exponentially decays in $|x|$, i.e., that there exist constants $C > 0$ and $k > 0$ such that

$$(8.18) \quad |u_\boldsymbol{\eta}(x)| \leq C e^{-k|x|}, \quad |u'_\boldsymbol{\eta}(x)| \leq C e^{-k|x|}, \quad |v_\boldsymbol{\eta}(x)| \leq C e^{k|x|}, \quad |v'_\boldsymbol{\eta}(x)| \leq C e^{k|x|}.$$

We can now give the proof of Lemma 8.2.

Proof of Lemma 8.2. The estimates (8.10) follow immediately from substituting formulas (8.14), (8.16), and (8.17) into (8.12) and applying the estimates (8.18). The estimates (8.11) follow by the same argument as in section 6. \square

It remains to prove Lemma 8.1.

Proof of Lemma 8.1. Directly setting $\boldsymbol{\zeta} = \boldsymbol{\eta}$ and substituting (8.14), (8.16), and (8.17) into (8.9) yields a long expression for $\mathcal{N}(\boldsymbol{\eta})$. To prove the claimed bound below, we note that the terms in this expression which depend quadratically on $v_\boldsymbol{\eta}(x)$ will dominate for sufficiently large M and hence we can ignore the other terms.

Regardless of whether $\Phi(0) \neq 0$ or $\Phi(0) = 0$, the terms which depend quadratically on v_η are

$$\begin{aligned}
 (8.19) \quad & - \left(v'_\eta(M) - i\sqrt{E}v_\eta(M) \right) \left(\int_0^{-M} u_\eta^2(y) \, dy \right) v'_\eta(-M) \\
 & + i\sqrt{E} \left(\int_0^{-M} u_\eta^2(y) \, dy \right) v_\eta(-M) \\
 & + \left(v'_\eta(-M) + i\sqrt{E}v_\eta(-M) \right) \left(\int_0^M u_\eta^2(y) \, dy \right) v'_\eta(M) \\
 & - i\sqrt{E} \left(\int_0^M u_\eta^2(y) \, dy \right) v_\eta(M),
 \end{aligned}$$

which simplifies to

$$\begin{aligned}
 (8.20) \quad & \int_{-M}^M u_\eta^2(y) \, dy \left(v'_\eta(M)v'_\eta(-M) - i\sqrt{E}v_\eta(M)v'_\eta(-M) \right. \\
 & \quad \left. + i\sqrt{E}v'_\eta(M)v_\eta(-M) + Ev_\eta(M)v_\eta(-M) \right) \\
 & = \int_{-M}^M u_\eta^2(y) \, dy \left(v'_\eta(M) - i\sqrt{E}v_\eta(M) \right) \left(v'_\eta(-M) + i\sqrt{E}v_\eta(-M) \right).
 \end{aligned}$$

Lemma 8.1 now follows since $\int_{-M}^M u_\eta^2(y) \, dy$ can be bounded below uniformly in M , and the two factors depending on v_η can be bounded below by Ce^{kM} exactly as in the proof of Lemma 5.2 (note that both factors $\neq 0$ since $v_\eta(x)$ is real, and see, in particular, (5.18)–(5.21)). \square

9. Further generalizations. In this section we describe further generalizations of our main result. In section 9.1 we study the case where a periodic structure hosting a defect state with $E < 0$ is truncated far from the defect, creating a new bound state whose associated eigenvalue is exponentially close to E . In Remark 9.1 we discuss the bound state created when a semi-infinite periodic structure hosting an edge state is truncated far from its edge.

9.1. One-dimensional defect states with negative energy $E < 0$ perturb to bound states of the truncated structure. We have so far assumed that the defect state eigenvalue is positive $E > 0$ throughout. In this section we again consider (2.1) in the simplest case, i.e., under Assumptions 2.1 and 2.2, but assume H has a bound state as in (2.4) but with negative energy $E < 0$ (the generalization when parity symmetry does not hold is straightforward along the same lines as when $E > 0$). Our aim is now to prove that when the structure modeled by H is truncated sufficiently far from $x = 0$, the resulting structure supports a bound state. More specifically, we will prove that the operator H_{trunc} defined by (2.5)–(2.6) has a bound state with energy $E^* < 0$ nearby to E for M sufficiently large (in particular, such that $M > \rho$, where ρ is the support of the defect region).

Let $u_z(x), X_1(z), X_2(z)$ be as in (2.8)–(2.9), and define $\Theta(z) := X_2(z) - i\sqrt{z}X_1(z)$. In contrast to (2.10), we now assume $z \in \mathbb{C} \setminus [0, \infty)$ and choose the branch of the square root such that $\text{Im} \sqrt{z} > 0$. With these definitions, $E^* < 0$ is a bound state whenever $\Theta(E^*) = 0$.

The counterpart of Theorem 2.1 in this context is as follows. Note that the theorem requires an additional assumption (9.1).

THEOREM 9.1. *Let $V(x)$ satisfy Assumptions 2.1 and 2.2, let Φ be a bound state with eigenvalue $E < 0$ as in (2.4), and let $v_z(x)$ be as in (2.13). Then there exist a $k > 0$ and an $M_0 > \rho \geq 0$ such that for all $M \geq M_0$ such that*

$$(9.1) \quad v'_E(M) - i\sqrt{E}v_E(M) \neq 0,$$

the following hold:

1. $\Theta(z)$ in (2.10) has a unique root E^* in ball $\Omega_M = \{z : |z - E| \leq \frac{1}{M^2}e^{-kM}\}$.
2. The root E^* is real and can be precisely characterized as

$$(9.2) \quad E^* = E - \frac{\Theta(E)}{\partial_z \Theta(E)} + O(e^{-4kM}).$$

Since the proof of Theorem 9.1 is so similar to that of Theorem 2.1, we omit it, although we point out the following:

- The condition (9.1) is also necessary for the proof of Theorem 2.1 when $E > 0$, but holds automatically because $v_E(x)$ is real for all x and in that case $i\sqrt{E}$ is purely imaginary. When $E < 0$, $i\sqrt{E} = i\sqrt{-|E|} = -\sqrt{|E|}$ is purely real.
- To see that the root $E^* < 0$ must be real, note that $\frac{\Theta(z)}{\partial_z \Theta(z)}$ is real for real and negative z and hence the map Ψ (3.1) actually maps $\mathbb{R} \rightarrow \mathbb{R}$ in this case.

Corollaries 2.2 and 2.3 directly generalize to this context. Since the results and proofs are identical after substituting $-\sqrt{|E|}$ for $i\sqrt{E}$, we omit them.

Remark 9.1. In recent years, bound states which decay away from the physical edge of a periodic structure known as edge states have attracted significant attention; see, e.g., [18, 20, 21, 28, 29, 30, 46]. These works generally assume the existence of a semi-infinite periodic structure adjoining the edge. Under an analogous assumption to (9.1), Theorem 9.1 should generalize easily to prove that the structure obtained by truncating the semi-infinite periodic structure far from the edge also hosts a bound state, with energy exponentially close (in the truncation distance) to the edge state energy. Note that the bound state of the truncated structure may not be exponentially small at the truncation; see [58].

Remark 9.2. The case $E = 0$ requires a specialized analysis which we do not undertake here. To see why our methods do not generalize, note for example that with $\Theta(z)$ defined by (2.10), the derivative $\partial_z \Theta(E)$ which appears in the definition of Ψ (3.1), and then in the formula for z^* (2.12), is not defined when $E = 0$.

10. Conclusions and perspectives. In this work we have studied the resonances created when periodic structures in one dimension hosting defect states are truncated far from the defect. Our results are restricted to one dimension because our methods rely on ODE theory, but there is no reason to expect that our results will not generalize to higher dimensions. Similarly, although our results are restricted to structures which are periodic away from a defect region because our methods rely on Floquet theory, we also expect our results will generalize to nonperiodic systems under appropriate spectral gap assumptions.

We can formulate a general conjecture regarding the resonances produced when a structure hosting a bound state is truncated away from the bound state maximum. Note that the existence of defect states in dimensions higher than 1 has been established across various models; see, e.g., [12, 32, 33, 37, 55].

CONJECTURE. *In \mathbb{R}^d , where d is an arbitrary positive integer, let H denote a Schrödinger operator $H := -\Delta + V$, where $V(\mathbf{x})$ has unbounded support. Assume*

that H hosts a bound state Φ whose eigenvalue E is isolated from the rest of the spectrum, i.e., $\sigma(H) \cap B_\rho(E) = \{E\}$, where $B_\rho(E)$ denotes a ball centered at E with positive radius $\rho > 0$. Let $\boldsymbol{\mu} := \int_{\mathbb{R}^d} \mathbf{x} |\Phi(\mathbf{x})|^2 d\mathbf{x}$ denote the center of mass of the bound state. Define $V_{trunc}(\mathbf{x})$ by

$$(10.1) \quad V_{trunc}(\mathbf{x}) = \begin{cases} V(\mathbf{x}), & \mathbf{x} \in B_M(\boldsymbol{\mu}), \\ 0, & \mathbf{x} \notin B_M(\boldsymbol{\mu}), \end{cases}$$

where $M > 0$, and define $H_{trunc} := -\Delta + V_{trunc}$. Then, for sufficiently large M , and assuming that Φ is nonzero for some $\mathbf{x} \notin B_M(\boldsymbol{\mu})$ (if not, Φ is a bound state of H_{trunc}), H_{trunc} will have a resonance z in the lower half of the complex plane such that $|z - E|$ is exponentially small in M .

Although the proofs in the present work rely on ODE theory, there is good reason to expect that such a result is true. First, exponential decay of bound states in gaps of essential spectrum in arbitrary dimensions follows under general hypotheses from exponential decay of the Green's function (see, e.g., [1, 11]). Second, in geometric scattering theory there are semiclassical methods for proving that classical orbits on manifolds or exterior to obstacles lead to resonances in the absence of any periodic background potential (see, e.g., Chap. 7 "From quasimodes to resonances" of Dyatlov and Zworski [26]). The methods developed there generalize the fixed point ODE tools used to demonstrate how eigenstates become resonances in the truncated harmonic oscillator that we have applied in the periodic setting. To study the defects to resonances question in higher-dimensional truncated lattice problems, one needs to develop similar tools, with the existence of a bound state of the infinite structure taking the place of the existence of trapped classical orbits in the semiclassical problem. Dobson et al. [16] have proved the conjecture in $d = 1$ for even potentials taking the form of large, constant barriers outside of a ball. Lin and Santosa [49] have proved in $d = 2$, again for potentials taking the form of large, constant barriers outside of a ball, that whenever a resonance occurs near to a bound state eigenvalue it must be exponentially close to the bound state eigenvalue. It would be interesting to generalize their approach, which uses Dirichlet-to-Neumann maps, to the general setting of our conjecture.

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