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Spectral properties of the Kronig–Penney Hamiltonian with a localized impurity

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It is shown that there exist bound states of the operator $H_{\pm\lambda} = -(d^2/dx^2) + \Sigma_{m\in Z}\delta(\cdot - (2m+1)\pi) \pm \lambda W$, W being an $L^1(-\infty, +\infty)$ non-negative function, in every sufficiently far gap of the spectrum of $H_0 = -d^2/dx^2 + \Sigma_{m\in Z}\delta(\cdot - (2m+1)\pi)$. Such an operator represents the Schrödinger Hamiltonian of a Kronig–Penney-type crystal with a localized impurity. The analyticity of the greatest (resp. lowest) eigenvalue of H_λ (resp. $H_{-\lambda}$) occurring in a spectral gap as a function of the coupling constant λ when W is assumed to have an exponential decay is also proven.

I. INTRODUCTION

In this paper we investigate some properties of the spectrum of the one-dimensional Schrödinger operator $H_{\pm\lambda} = H_0 \pm \lambda W$ with $\lambda > 0$,

$$H_0 = -\frac{d^2}{dx^2} + \sum_{m\in Z}\delta(\cdot - (2m+1)\pi)$$

and W being a non-negative L^1 function.

The Hamiltonian represents the Kronig–Penney model of a crystal with a localized impurity given by the short-range potential W.

There have been several papers[1–5] investigating the spectrum of the operator $H_{\pm\lambda}$ when H_0 is the Schrödinger Hamiltonian with a piecewise continuous periodic potential. In Ref. 6 the case of a nonperiodic potential V having a "short-range" order, so that $H_0 = d^2/dx^2 + V$ still has gaps in its spectrum, is studied. The main tool in our analysis will be the Birman–Schwinger kernel. Furthermore, we will exploit the Gel'fand expansion for the resolvent of H_0 (see Refs. 7 and 8) in order to have a convenient expression for the Birman–Schwinger kernel.

By doing so we show that there is a band in the spectrum of H_0 such that there exist eigenvalues of $H_{\pm\lambda}$ in each gap on the right of that band and if λ is sufficiently small we can find eigenvalues in each gap of $\sigma(H_0) = \sigma_{\text{ess}}(H_{\pm\lambda})$.

Furthermore, we prove that under the stronger assumption of an exponential falloff of W, the greatest (resp. lowest) eigenvalue of $H_{+\lambda}$ (resp. $H_{-\lambda}$) occurring in a spectral gap is analytic as a function of the coupling constant λ.

The other important problem related to the asymptotics of the number of bound states in each gap will be studied in another paper.

II. BOUND STATES OF $H_0 \pm \lambda W$ IN THE GAPS OF $\sigma(H_0)$

In this section we shall be concerned with the existence of bound states of $H_0 \pm \lambda W$ inside the gaps of $\sigma(H_0)$.

First of all, let us recall that the spectrum of the unperturbed Hamiltonian H_0 is given by

$$\sigma(H_0) = \left(\bigcup_{k=0}^{\infty}[E_{2k+1}(0), (k+\tfrac{1}{2})^2]\right) \cup \left(\bigcup_{k=1}^{\infty}[E_{2k}(\pi), k^2]\right),$$

$E_n(\theta)$ being the nth root of the well-known Kronig–Penney equation

$$\cos 2\pi\sqrt{E} + (1/2\sqrt{E})\sin 2\pi\sqrt{E} = \cos\theta \qquad (2.1)$$

with $\theta\in[0,\pi]$ (see Ref. 9).

For each fixed θ, $\{E_n(\theta)\}_{n=1}^{\infty}$ are the eigenvalues of the reduced Hamiltonian $H_0(\theta) = (-d^2/dx^2)_\theta + \delta(\cdot - \pi)$ whose eigenfunctions are given by

$$\phi_n^{(\theta)}(x) = A_n^{(\theta)}\begin{cases}\cos\sqrt{E_n(\theta)}\,x \\ \quad -((1-e^{i\theta}/1+e^{i\theta}))\cot\sqrt{E_n(\theta)}\,\pi\sin\sqrt{E_n(\theta)}\,x, & 0\leqslant x\leqslant\pi, \\ e^{i\theta}\left[\cos\sqrt{E_n(\theta)}\,(x-2\pi)\right. \\ \quad \left. -((1-e^{i\theta}/1+e^{i\theta}))\cot\sqrt{E_n(\theta)}\,\pi\sin\sqrt{E_n(\theta)}\,(x-2\pi)\right], & \pi\leqslant x\leqslant 2\pi,\end{cases} \qquad (2.2)$$

$A_n^{(\theta)}$ being the normalization constant.

In the particular cases when $\theta = 0$, $\theta = \pi$ the eigenfunctions can be written as

$$\phi_{2k+1}^{(0)}(x) = \left(\pi + \frac{\sin 2\pi\sqrt{E_{2k+1}(0)}}{2\sqrt{E_{2k+1}(0)}}\right)^{-1}\begin{cases}\cos\sqrt{E_{2k+1}(0)}\,x, & 0\leqslant x\leqslant\pi, \\ \cos\sqrt{E_{2k+1}(0)}\,(x-2\pi), & \pi\leqslant x\leqslant 2\pi,\end{cases} \qquad (2.3)$$

$$\phi_{2k}^{(0)}(x) = (1/\sqrt{2\pi}) \sin kx \tag{2.4}$$

and

$$\phi_{2k+1}^{(\pi)}(x) = (1/\sqrt{2\pi}) \cos(k + \tfrac{1}{2})x, \tag{2.5}$$

$$\phi_{2k}^{(\pi)}(x) = \left(\pi - \frac{\sin 2\pi\sqrt{E_{2k}(\pi)}}{2\sqrt{E_{2k}(\pi)}}\right)^{-1} \times \begin{cases} \sin\sqrt{E_{2k}(\pi)}x, & 0 \leqslant x \leqslant \pi, \\ \sin\sqrt{E_{2k}(\pi)}(2\pi - x), & \pi \leqslant x \leqslant 2\pi. \end{cases} \tag{2.6}$$

By means of some boring algebra we can determine the normalization constant $A_n^{(\theta)}$, precisely

$$A_n^{(\theta)} = \left[\pi + \frac{\sin 2\pi\sqrt{E_n(\theta)}}{2\sqrt{E_n(\theta)}} + \left(\frac{1-\cos\theta}{1+\cos\theta}\right) \times \cot^2 \pi\sqrt{E_n(\theta)}\left(\frac{\sin 2\pi\sqrt{E_n(\theta)}}{2\sqrt{E_n(\theta)}}\right)\right]^{-1/2}. \tag{2.7}$$

This immediately leads to the following result whose proof is omitted since it only consists of tedious calculations.

Lemma 2.1: Let $\phi_n^{(\theta)}$ be the nth eigenfunction of the reduced Hamiltonian $H_0(\theta) = (-d^2/dx^2)_\theta + \delta(\cdot - \pi)$ acting on $L^2[0,2\pi]$ with $\theta \in [0,\pi]$. Then the following estimate holds:

$$\|\phi_n^{(\theta)}\|_\infty \leqslant \frac{1}{\sqrt{\pi}}\left[1 - \left(\frac{\sin 2\pi\sqrt{E_1(0)}}{2\pi\sqrt{E_1(0)}}\right)^2\right]^{-1/2} \tag{2.8}$$

for any $n \in N$ and any $\theta \in [0,\pi]$.

Remark: Since $\phi_n^{(2\pi-\theta)} = \overline{\phi_n^{(\theta)}}$, because of the antiunitarity of $H_0(\theta)$ and $H_0(\theta - 2\pi)$, the estimate (2.8) actually holds for any $\theta \in [0,2\pi]$. We shall use this property later.

After these preliminaries we consider the Birman–Schwinger operator in our particular case. Since W is a definite-sign function our Birman–Schwinger operator is self-adjoint. It is not difficult to show that $W^{1/2}(H_0 - E)^{-1}W^{1/2}$ ($W \geqslant 0$) is trace class for any $E \in \rho(H_0)$. One can first prove that this holds for $E < 0$ since

$$\|W^{1/2}(H_0 - E)^{-1}W^{1/2}\|_1 \leqslant \|W^{1/2}\left(-\frac{d^2}{dx^2} - E\right)^{-1}W^{1/2}\|_1 \tag{2.9}$$

for any $E < 0$.

Then, by using the first resolvent equation and the connectedness of the resolvent set of H_0, it follows that the property holds for any $E \in \rho(H_0)$.

This implies that we are allowed to use the KLMN theorem (see Refs. 10 and 11) in order to define the self-adjoint operator whose quadratic form is given by

$$(\psi,(H_0 \pm \lambda W)\psi) = (\psi, H_0\psi) \pm \lambda(\psi, W\psi)$$

for any $\psi \in Q(H_0)$.

Furthermore, we can apply the Fredholm theory to our Birman-Schwinger kernel. In particular, we can see that if $W \geqslant 0$, E is an eigenvalue of $H_0 \pm \lambda W$ if and only if ∓ 1 is an eigenvalue of $\lambda W^{1/2}(H_0 - E)^{-1}W^{1/2}$.

In order to obtain some information about the eigenvalues of $W^{1/2}(H_0 - E)^{-1}W^{1/2}$ when E belongs to some gap of $\sigma(H_0)$, we express the BS kernel by means of the Gel'fand transform, namely,

$$W^{1/2}(H_0 - E)^{-1}W^{1/2} = \sum_{n=1}^{\infty} \int_0^{2\pi} \frac{|W^{1/2}\phi_n^{(\theta)}\rangle\langle W^{1/2}\phi_n^{(\theta)}|}{E_n(\theta) - E} \frac{d\theta}{2\pi} \tag{2.10}$$

($\phi_n^{(\theta)}$ having been extended to the whole real axis by means of the θ condition), which makes sense for any $E \in \rho(H_0)$ because of Lemma 2.1 and the fact that $W \in L^1(R)$ as written in the Introduction.

If $E \in (-\infty, E_1(0))$, $W^{1/2}(H_0 - E)^{-1}W^{1/2}$ is a positive operator which implies that only $H_0 - \lambda W$ can have bound states lying in $(-\infty, E_1(0))$.

If E lies inside a gap the series on the rhs of (2.10) gives rise to a negative term in the expectation value of the BS kernel with respect to ψ due to the integrals related to the bands on the left of the gap containing E. For simplicity, let us only consider the case related to $H_0 - \lambda W$.

For our specific purpose we can neglect the negative term related to

$$W^{1/2}(H_0 - E)_-^{-1} W^{1/2} = -\sum_{n=1}^{2N} \int_0^{2\pi} \frac{|W^{1/2}\phi_n^{(\theta)}\rangle\langle W^{1/2}\phi_n^{(\theta)}|}{E - E_n(\theta)} \frac{d\theta}{2\pi} \tag{2.11}$$

since it can only lower the eigenvalues of the positive operator

$$W^{1/2}(H_0 - E)_+^{-1}W^{1/2} \tag{2.12}$$

similarly defined.

At this point we can start our analysis about the bound states of $H_0 - \lambda W$. First of all, we show the existence of bound states of $H_0 - \lambda W$ in every sufficiently far gap of $\sigma(H_0)$.

Theorem 2.2: Let

$$H_0 = -\frac{d^2}{dx^2} + \sum_{m=-\infty}^{+\infty} \delta(\cdot - (2m+1)\pi)$$

and W be a positive function belonging to $L^1(R)$. Then, for any fixed $\lambda > 0$, there exists a certain band of $\sigma(H_0)$ such that every gap on the right of that band contains eigenvalues of $H_\lambda = H_0 - \lambda W$.

Proof: First of all, we notice that the integral related to the $(2N+1)$st band in the expression of $W^{1/2}(H_0 - E)_+^{-1}W^{1/2}$ diverges when $E \to E_{2N+1}(0)_-$ on the one-dimensional subspace $\{W^{1/2}\phi_{2N+1}^{(0)}\}$.

Therefore the norm of $W^{1/2}(H_0 - E)_+^{-1}W^{1/2}$ increases without limit when $E \to E_{2N+1}(0)_-$.

Since this operator is compact and positive its greatest eigenvalue is equal to the norm of the operator. If $\lambda\|W^{1/2}(H_0 - N^2)_+^{-1}W^{1/2}\| < 1$, there must be an $\tilde{E} \in (N^2, E_{2N+1}(0))$ such that $\lambda W^{1/2}(H_0 - \tilde{E})^{-1}W^{1/2}\psi = \psi$, for some $\psi \in L^2(R)$. Of course, a completely similar analysis can be carried out when $E \in ((N+\tfrac{1}{2})^2, E_{2(N+1)}(\pi))$ for any fixed N. Therefore we need to show that $\|W^{1/2}(H_0 - N^2)_+^{-1}W^{1/2}\| \to 0$ when $N \to +\infty$.

For any ψ we have

$$(\psi, W^{1/2}(H_0-N^2)_+^{-1}W^{1/2}\psi)$$
$$=\sum_{n=2N+1}^{\infty}\int_0^{2\pi}\frac{|(W^{1/2}\phi_n^{(\theta)},\psi)|^2}{E_n(\theta)-N^2}\frac{d\theta}{2\pi}$$
$$\leqslant\frac{\|W\|_1\|\psi\|_2^2}{2\pi^2}\left[1-\left(\frac{\sin 2\pi\sqrt{E_1(0)}}{2\pi\sqrt{E_1(0)}}\right)^2\right]^{-1}$$
$$\times\left(\sum_{n=2N+1}^{\infty}\int_0^{2\pi}\frac{1}{E_n(\theta)-N^2}d\theta\right). \tag{2.13}$$

At this point we must prove that the series on the rhs of (2.13) goes to zero as N goes to infinity. First of all, let us consider

$$\sum_{n=2(N+1)}^{\infty}\int_0^{2\pi}\frac{1}{E_n(\theta)-N^2}d\theta. \tag{2.14}$$

The term with $n=2N+1$ will be considered later.

We can bound each integral in the series by replacing $E_n(\theta)$ by means of $E_{2k}(0)$ if $n=2k+1$ or $E_{2k-1}(\pi)$ if $n=2k$.

Hence

$$(2.14)\leqslant 2\pi\left(\sum_{n=0}^{\infty}\frac{1}{(n+\frac{1}{2})(2N+n+\frac{1}{2})}\right.$$
$$\left.+\sum_{n=0}^{\infty}\frac{1}{(n+1)(2N+n+1)}\right). \tag{2.15}$$

Since for any fixed N

$$\left\{\frac{1}{(n+\frac{1}{2})(2N+n+\frac{1}{2})}\right\}_{n=0}^{\infty}$$

and

$$\left\{\frac{1}{(n+1)(2N+n+1)}\right\}_{n=0}^{\infty}$$

are l_1 sequences dominated by

$$\left\{\frac{1}{(n+\frac{1}{2})^2}\right\}_{n=0}^{\infty}\in l_1,$$

by means of the dominated convergence theorem we get that the rhs of (2.15) goes to zero as $N\to\infty$.

In order to complete the proof of the theorem we only need to prove that

$$\int_0^{2\pi}\frac{1}{E_{2N+1}(\theta)-N^2}d\theta$$
$$=2\int_0^{\pi}\frac{1}{E_{2N+1}(\theta)-N^2}d\theta\to 0 \tag{2.16}$$

as $N\to\infty$.

For any $0<\epsilon<\pi$ we have

$$\int_0^{\epsilon}\frac{1}{E_{2N+1}(\theta)-N^2}d\theta+\int_{\epsilon}^{\pi}\frac{1}{E_{2N+1}(\theta)-N^2}d\theta$$
$$\leqslant\frac{\epsilon}{E_{2N+1}(0)-N^2}+\frac{\pi-\epsilon}{E_{2N+1}(\epsilon)-N^2} \tag{2.17}$$

since $E_{2N+1}(\theta)$ is an increasing function of θ (see Ref. 12).

By applying Taylor's theorem with remainder to (2.1) near $\sqrt{E}=\sqrt{E_{2N+1}(0)}$ we get

$$\cos 2\pi\sqrt{E_{2N+1}(0)}+\frac{1}{2\sqrt{E_{2N+1}(0)}}\sin 2\pi\sqrt{E_{2N+1}(0)}$$
$$-\left[\left(2\pi+\frac{1}{2\tilde{E}_{2N+1}}\right)\sin 2\pi\sqrt{\tilde{E}_{2N+1}}\right.$$
$$\left.-\frac{\pi}{\sqrt{\tilde{E}_{2N+1}}}\cos 2\pi\sqrt{\tilde{E}_{2N+1}}\right]$$
$$\times(\sqrt{E_{2N+1}(\theta)}-\sqrt{E_{2N+1}(0)})=\cos\theta \tag{2.18}$$

[with $\tilde{E}_{2N+1}\in(E_{2N+1}(0),E_{2N+1}(\theta))$], which implies that for $\theta=\epsilon$

$$\sqrt{E_{2N+1}(\epsilon)}-\sqrt{E_{2N+1}(0)}$$
$$\geqslant\frac{1-\cos\epsilon}{2\pi+\pi/\sqrt{E_{2N+1}(0)}+1/E_{2N+1}(0)}$$
$$\geqslant\frac{1}{4\pi}(1-\cos\epsilon) \tag{2.19}$$

for N large, since

$$\cos 2\pi\sqrt{E_{2N+1}(0)}+[2E_{2N+1}(0)]^{-1}$$
$$\times\sin 2\pi\sqrt{E_{2N+1}(0)}=1.$$

Thus we obtain

$$([E_{2N+1}(\epsilon)-E_{2N+1}(0)]+E_{2N+1}(0)-N^2)^{-1}$$
$$\leqslant([E_{2N+1}(0)/2\pi](1-\cos\epsilon)$$
$$+[E_{2N+1}(0)-N^2])^{-1}, \tag{2.20}$$

which implies

$$(\pi-\epsilon)/[E_{2N+1}(\epsilon)-N^2]\to 0 \tag{2.21}$$

as $N\to\infty$ for any $0<\epsilon<\pi$ since $\lim_{N\to\infty}[E_{2N+1}(0)-N^2]=1/\pi$ (see Ref. 12).

Therefore, for any $0<\epsilon<\pi$, we have

$$\lim_{N\to\infty}\int_0^{\pi}\frac{1}{E_{2N+1}(\theta)-N^2}d\theta$$
$$\leqslant\lim_{N\to\infty}\frac{\epsilon}{E_{2N+1}(0)-N^2}=\pi\epsilon \tag{2.22}$$

which gives (2.16). Q.E.D.

As a consequence of Theorem 2.2, we have the following corollary.

Corollary 2.3: If

$$\lambda<\frac{\pi[1-(\sin 2\pi\sqrt{E_1(0)}/2\pi\sqrt{E_1(0)})^2]}{\|W\|_1[(\inf_{1<n<\infty}[a_{n+1}-b_n])^{-1}+2\Sigma_{n=0}^{\infty}((n+\frac{1}{2})^2)^{-1}]} \tag{2.23}$$

[(b_n, a_{n+1}) being the nth gap of $\sigma(H_0)$] and with the same assumptions of Theorem 2.2, $H_0 - \lambda W$ has eigenvalues in every gap of $\sigma(H_0)$ (the inf is different from zero since there are no connected bands and $a_{n+1} - b_n$ converges to π^{-1} as follows from the analysis in Ref. 12).

Proof: From (2.13) and (2.15) we get

$$\lambda \|W^{1/2}(H_0 - N^2)_+^{-1} W^{1/2}\|$$

$$\leqslant \lambda \frac{\|W\|_1}{\pi}\left[1 - \left(\frac{\sin 2\pi\sqrt{E_{2N+1}(0)}}{2\pi\sqrt{E_{2N+1}(0)}}\right)^2\right]^{-1}$$

$$\times\left[\frac{1}{E_{2N+1}(0) - N^2} + 2\sum_{n=0}^{\infty}\frac{1}{(n+\frac{1}{2})^2}\right], \quad (2.24)$$

which is less than one for any N since λ satisfies (2.23). By means of similar estimates we obtain the same result for the gaps of the type $((N-\frac{1}{2})^2, E_{2N}(\pi))$. Q.E.D.

Of course, completely similar results hold in the case of $H_0 + \lambda W$. At this point we are going to investigate the behavior of the eigenvalues of $H_0 + \lambda W$ occurring in the gaps of $\sigma(H_0)$ for small values of the coupling constant λ.

III. COUPLING CONSTANT THRESHOLD BEHAVIOR FOR $H_0 - \lambda W$ AT $\lambda = 0$

In this section we are going to show that in the case of a non-negative potential W having an exponential falloff $\tilde{E}_{2N+1}(\lambda)$, the smallest eigenvalue of $H_0 - \lambda W$ inside the spectral gap $(E_{2N}(0), E_{2N+1}(0))$, is an analytic function of λ at $\lambda = 0$. First of all, we notice that

$$\lim_{\lambda \to 0} \tilde{E}_{2N+1}(\lambda) = E_{2N+1}(0),$$

since $H_0 - \lambda W \to H_0$ as $\lambda \to 0$ in the norm resolvent sense [in the case of the gap $((N-\frac{1}{2})^2, E_{2N}(\pi))$, $\tilde{E}_{2N}(\lambda)$ clearly converges to $E_{2N}(\pi)$].

In order to show the analyticity of $\tilde{E}_{2N+1}(\lambda)$ at $\lambda = 0$ we shall follow the strategy used in Ref. 8 (p. 337) since we know that $E \in (E_{2N}(0), E_{2N+1}(0))$ is an eigenvalue of $H_0 - \lambda W$ if and only if

$$\det(I - \lambda W^{1/2}(H_0 - E)^{-1} W^{1/2}) = 0. \quad (3.1)$$

First of all, the BS kernel can be expressed as follows:

$$W^{1/2}(H_0 - E)^{-1} W^{1/2} = M_E^{(1)} + M_E^{(2)} + \frac{1}{2\pi}\left(\int_0^{2\pi}\frac{1}{E_{2N+1}(\theta) - E}\,d\theta\right) \times |W^{1/2}\phi_{2N+1}^{(0)}\rangle\langle W^{1/2}\phi_{2N+1}^{(0)}| \quad (3.2)$$

with

$$M_E^{(1)} = \int_0^{2\pi}\frac{|W^{1/2}\phi_{2N+1}^{(\theta)}\rangle\langle W^{1/2}\phi_{2N+1}^{(\theta)}| - |W^{1/2}\phi_{2N+1}^{(0)}\rangle\langle W^{1/2}\phi_{2N+1}^{(0)}|}{E_{2N+1}(0) - E}\frac{d\theta}{2\pi} \quad (3.3)$$

and

$$M_E^{(2)} = \sum_{n \neq 2N+1}\int_0^{2\pi}\frac{|W^{1/2}\phi_n^{(\theta)}\rangle\langle W^{1/2}\phi_n^{(\theta)}|}{E_n(\theta) - E}\frac{d\theta}{2\pi}. \quad (3.4)$$

First of all, we notice that the operator-valued function $M_E^{(2)}$ is analytic at $E = E_{2N+1}(0)$. At this point we are going to show the boundedness of $M_{E_{2N+1}(0)}^{(1)}$ under a suitable assumption on W.

Proposition 3.1: If $W^{1/2} \in D(x^2)$ then $M_{E_{2N+1}(0)}^{(1)}$ is a bounded operator on $L^2(-\infty, +\infty)$.

Proof: First of all, the integral expression $M_{E_{2N+1}(0)}^{(1)}$ can be written in a more convenient form by using the antiunitarity of the operators $H_0(\theta)$ and $H_0(2\pi - \theta)$, i.e.,

$$M_{E_{2N+1}(0)}^{(1)} = \int_0^{\pi}\frac{|W^{1/2}\,\overline{\phi_{2N+1}^{(\theta)}}\rangle\langle W^{1/2}\,\overline{\phi_{2N+1}^{(\theta)}}| + |W^{1/2}\,\phi_{2N+1}^{(\theta)}\rangle\langle W^{1/2}\,\overline{\phi_{2N+1}^{(\theta)}}| - 2|W^{1/2}\,\overline{\phi_{2N+1}^{(0)}}\rangle\langle W^{1/2}\,\overline{\phi_{2N+1}^{(0)}}|}{E_{2N+1}(\theta) - E_{2N+1}(0)}\frac{d\theta}{2\pi}, \quad (3.5)$$

which can also be written

$$2\int_0^{2\pi}\frac{|W^{1/2}\Re\phi_{2N+1}^{(\theta)}\rangle\langle W^{1/2}\Re\phi_{2N+1}^{(\theta)}| + |W^{1/2}\Im\phi_{2N+1}^{(\theta)}\rangle\langle W^{1/2}\Im\phi_{2N+1}^{(\theta)}| - |W^{1/2}\phi_{2N+1}^{(0)}\rangle\langle W^{1/2}\phi_{2N+1}^{(0)}|}{E_{2N+1}(\theta) - E_{2N+1}(0)}\frac{d\theta}{2\pi}. \quad (3.6)$$

At this point we want to show that the norm of the operator defined by (3.6) is finite. From the Kronig–Penney relation we know that the function $E_{2N+1}(\theta) - E_{2N+1}(0)$ has only a zero at $\theta = 0$.

Furthermore, $E_{2N+1}(\theta) - E_{2N+1}(0)$ goes to zero like θ^2 when θ goes to zero since $E_{2N+1}(\theta)$ is an even function and

$$\frac{d^2 E_{2N+1}(\theta)}{d\theta^2}\Big|_{\theta=0} > 0 \quad (3.7)$$

as can be seen by computing the implicit function derivative by means of the Kronig–Penney relation.

Therefore $\theta = 0$ is a removable singularity for the function $\theta^{-2}[E_{2N+1}(\theta) - E_{2N+1}(0)]$ which implies also

$$\inf_{\theta \in [0,\pi]}\theta^{-2}[E_{2N+1}(\theta) - E_{2N+1}(0)] > 0 \quad (3.8)$$

since the function has no zeros in $[0,\pi]$.

Consequently the operator norm of (3.6) is bounded by

$$2\Big(\inf_{\theta\in[0,\pi]}\theta^{-2}[E_{2N+1}(\theta)-E_{2N+1}(0)]\Big)$$
$$\times\Big\|\int_0^\pi \theta^{-2}[|W^{1/2}\Re\phi_{2N+1}^{(\theta)}\rangle\langle W^{1/2}\Re\phi_{2N+1}^{(\theta)}|+|W^{1/2}\Im\phi_{2N+1}^{(\theta)}\rangle$$
$$\times\langle W^{1/2}\Im\phi_{2N+1}^{(\theta)}|-|W^{1/2}\phi_{2N+1}^{(0)}\rangle\langle W^{1/2}\phi_{2N+1}^{(0)}|]\frac{d\theta}{2\pi}\Big\|. \tag{3.9}$$

Since $\Re\phi_{2N+1}^{(\theta)}$ and $\Im\phi_{2N+1}^{(\theta)}$ are real analytic functions of θ we have the following McLaurin expansions:

$$\Im\phi_{2N+1}^{(\theta)}=\left[\frac{d}{d\theta}\Im\phi_{2N+1}^{(\theta)}\right]_{\theta=\tilde\theta}\theta \tag{3.10}$$

for some $\tilde\theta\in(0,\theta)$ and

$$\Re\phi_{2N+1}^{(\theta)}=\phi_{2N+1}^{(0)}+\left[\frac{d^2}{d\theta^2}\Re\phi_{2N+1}^{(\theta)}\right]_{\theta=\theta^*}\frac{\theta^2}{2} \tag{3.11}$$

for some $\theta^*\in(0,\theta)$.

Therefore (3.9) becomes

$$2\Big(\inf_{\theta\in[0,\pi]}\theta^{-2}[E_{2N+1}(\theta)-E_{2N+1}(0)]\Big)\Big\|\int_0^\pi\Big[\Big|W^{1/2}\Big[\frac{d}{d\theta}\Im\phi_{2N+1}^{(\theta)}\Big]_{\theta=\tilde\theta}\Big\rangle\Big\langle W^{1/2}\Big[\frac{d}{d\theta}\Im\phi_{2N+1}^{(\theta)}\Big]_{\theta=\tilde\theta}\Big|$$
$$+\frac{1}{2}\Big(|W^{1/2}\phi_{2N+1}^{(0)}\rangle\Big\langle W^{1/2}\Big[\frac{d^2}{d\theta^2}\Re\phi_{2N+1}^{(\theta)}\Big]_{\theta=\theta^*}\Big|+\Big|W^{1/2}\Big[\frac{d^2}{d\theta^2}\Re\phi_{2N+1}^{(\theta)}\Big]_{\theta=\theta^*}\Big\rangle\langle W^{1/2}\phi_{2N+1}^{(\theta)}|\Big)$$
$$+\frac{\theta^2}{4}\Big|W^{1/2}\Big[\frac{d^2}{d\theta^2}\Re\phi_{2N+1}^{(\theta)}\Big]_{\theta=\theta^*}\Big\rangle\Big\langle W^{1/2}\Big[\frac{d^2}{d\theta^2}\Re\phi_{2N+1}^{(\theta)}\Big]_{\theta=\theta^*}\Big|\Big\rangle\frac{d\theta}{2\pi}\Big\|. \tag{3.12}$$

By using the explicit expression of $\phi_n^{(\theta)}$ given in Sec. II, it is not difficult to show that there are two positive constants $A_1^{(N)}, B_1^{(N)}$ such that

$$\left|\frac{d}{d\theta}\Im\phi_{2N+1}^{(\theta)}(x)\right|\leqslant A_1^{(N)}|x|+B_1^{(N)}$$

for any real x and any $\theta\in[0,\pi)$. Similarly we have

$$\left|\frac{d^2}{d\theta^2}\Re\phi_{2N+1}^{(\theta)}(x)\right|\leqslant A_2^{(N)}x^2+B_2^{(N)}|x|+C^{(N)}$$

for some positive constants $A_2^{(N)}, B_2^{(N)}, C^{(N)}$.

These estimates together with our assumption on $W^{1/2}$ imply that the operator-valued integral inside the norm in (3.12) has norm bounded by

$$2\int_0^\pi\Big[\|W^{1/2}(A_1^{(N)}|x|+B_1^{(N)})\|_2^2+\|W^{1/2}\phi_{2N+1}^{(0)}\|_2\|W^{1/2}(A_2^{(N)}x^2+B_2^{(N)}|x|+C^{(N)})\|_2$$
$$+\frac{\theta^2}{4}\|W^{1/2}(A_2^{(N)}x^2+B_2^{(N)}|x|+C^{(N)}\|_2^2\Big]\frac{d\theta}{2\pi}<\infty, \tag{3.13}$$

which completes the proof of the proposition. Q.E.D.

Since $M_E^{(1)}$ and $M_E^{(2)}$ are both bounded at $E=E_{2N+1}(0)$ it follows that, if $E(\lambda)$ is a solution of (3.1) with the BS kernel given by (3.2), $[I-\lambda(M_{E(\lambda)}^{(1)}+M_{E(\lambda)}^{(2)})]$ is invertible for any λ sufficiently small. Therefore, following Ref. 8, we only need to study the equation

$$\det\Big[I-\frac{\lambda}{2\pi}\Big(\int_0^{2\pi}\frac{1}{E_{2N+1}(\theta)-E}d\theta\Big)|W^{1/2}\phi_{2N+1}^{(0)}\rangle$$
$$\times\langle W^{1/2}\phi_{2N+1}^{(0)}|[I-\lambda(M_E^{(1)}+M_E^{(2)})]^{-1}\Big]=0. \tag{3.14}$$

Since for any rank 1 operator B we have $\det(1+B)=1+\mathrm{Tr}(B)$, (3.14) becomes

$$1-\frac{\lambda}{2\pi}\Big(\int_0^{2\pi}\frac{1}{E_{2N+1}(\theta)-E}d\theta\Big)(W^{1/2}\phi_{2N+1}^{(0)},$$
$$[I-\lambda(M_E^{(1)}+M_E^{(2)})]^{-1}W^{1/2}\phi_{2N+1}^{(0)})=0. \tag{3.15}$$

At this point we state and prove the main theorem of this section.

Theorem 3.2: Let H_0 be the Kronig–Penney Hamiltonian. If $W \geqslant 0$ and $W^{1/2} \in D(e^{\alpha|x|})$ for some $\alpha > 0$, then (a) $\tilde{E}_n(\lambda)$, the smallest eigenvalue of $H_0 - \lambda W$ in the spectral gap $(E_{n-1}(0), E_n(0))$ for n odd, $(E_{n-1}(\pi), E_n(\pi))$ for n even, is analytic at $\lambda = 0$ and

$$\tilde{E}_n(\lambda) = \tilde{E}_n - \frac{\widetilde{m}_n^*}{2}\left(\int_{-\infty}^{\infty} W(x)[\tilde{\phi}_n(x)]^2\, dx\right)^2 \lambda^2 + o(\lambda^2), \tag{3.16}$$

where

$$\tilde{E}_n = \begin{cases} E_n(0), & n = 2k+1, \\ E_n(\pi), & n = 2k, \end{cases}$$

$$m_n^* = \begin{cases} m_n^*(0), & n = 2k+1, \\ m_n^*(\pi), & n = 2k, \end{cases}$$

$$\tilde{\phi}_n(x) = \begin{cases} \phi_n^{(0)}(x), & n = 2k+1, \\ \phi_n^{(\pi)}(x), & n = 2k, \end{cases}$$

$m_n^*(\theta)$ being the effective mass; (b) $\lambda = 0$ is a coupling constant threshold.

Proof: By setting $E = E(\eta) = E_{2N+1}(0) - \eta^2$, $\eta > 0$ and multiplying both sides of Eq. (3.15) by η we get the equation

$$\eta - \frac{\lambda}{2\pi}\left(\int_0^{2\pi} \frac{\eta}{[E_{2N+1}(\theta) - E_{2N+1}(0)] + \eta^2}\, d\theta\right)$$
$$\times (W^{1/2}\phi_{2N+1}^{(0)}, [I - \lambda(M_{E(\eta)}^{(1)} + M_{E(\eta)}^{(2)})]^{-1} W^{1/2}\phi_{2N+1}^{(0)}) = 0. \tag{3.17}$$

Thus we must show the existence of the function $\eta(\lambda)$ solution of Eq. (3.17) in a neighborhood of $\lambda = 0$ and its analyticity at $\lambda = 0$.

In order to achieve this result we shall use the implicit function theorem applied to Eq. (3.17). Therefore we have to prove that $F(\eta,\lambda)$ given by the left-hand side of Eq. (3.17) is jointly analytic in η and λ at $\langle \eta,\lambda \rangle = \langle 0,0 \rangle$ and that $F(\eta,\lambda)$ satisfies the conditions $F(0,0) = 0$, $(\partial F/\partial \eta)_0 \neq 0$.

First of all, we notice that $M_{E(\eta)}^{(2)}$ is an analytic function of η at 0 since

$$(\psi, M_{E(\eta)}^{(2)}\psi) = \sum_{n \neq 2N+1} \int_0^{2\pi} \frac{|(\psi, W^{1/2}\phi_n^{(\theta)})|^2}{[E_n(\theta) - E_{2N+1}(0)] + \eta^2} \frac{d\theta}{2\pi} \tag{3.18}$$

is an analytic function of η at $\eta = 0$ for any $\psi \in L^2(R)$ which implies the analyticity of the operator-valued function $M_{E(\eta)}^{(2)}$ (see Ref. 13 for the relation between analyticity in the weak operator topology and norm analyticity). Now we must show the analyticity of the functions

$$f(\eta) = \int_0^{2\pi} \frac{\eta}{[E_{2N+1}(\theta) - E_{2N+1}(0)] + \eta^2}\, d\theta$$

and

$$M_{E(\eta)}^{(1)} = \int_0^{2\pi} \frac{|W^{1/2}\phi_{2N+1}^{(\theta)}\rangle\langle W^{1/2}\phi_{2N+1}^{(\theta)}| - |W^{1/2}\phi_{2N+1}^{(0)}\rangle\langle W^{1/2}\phi_{2N+1}^{(0)}|}{[E_{2N+1}(\theta) - E_{2N+1}(0)] + \eta^2} \frac{d\theta}{2\pi}$$

at $\eta = 0$.

Let us begin by considering the first integral which can also be written as

$$\int_{-\pi}^{\pi} \frac{\eta}{g^2(\theta) + \eta^2} \frac{d\theta}{2\pi}$$

with

$$g^2(\theta) = E_{2N+1}(\theta) - E_{2N+1}(0) = \sum_{l=1}^{\infty} \beta_{2l}\theta^{2l}.$$

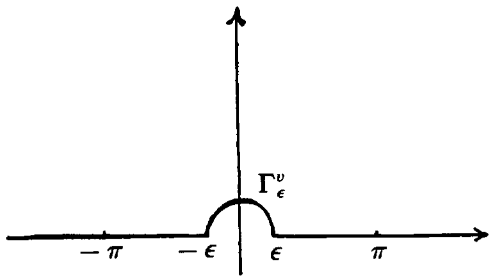
Furthermore

$$\int_{-\pi}^{\pi} \frac{\eta}{g^2(\theta) + \eta^2} \frac{d\theta}{2\pi} = \frac{i}{4\pi}\left[\int_{-\pi}^{\pi} \frac{1}{g(\theta) + i\eta}\, d\theta - \int_{-\pi}^{\pi} \frac{1}{g(\theta) - i\eta}\, d\theta\right]. \tag{3.19}$$

First of all, we note that $g(\theta)$ is real analytic and has an analytic extension to a complex neighborhood of $(-\pi,\pi)$.

If $\eta > 0$ the singularity of $1/[g(\theta) + i\eta]$ is located in the lower half-plane as can be seen by noticing that the leading term of the MacLaurin expansion of $g(\theta)$ is given by $\beta_2^{1/2}\theta$ with $\beta_2^{1/2} > 0$ and therefore the solution of $g(\theta) = -i\eta$ lies on the negative imaginary semiaxis.

Thus we can choose the path of integration shown below



and we have

$$\int_{-\pi}^{\pi} \frac{1}{g(\theta) + i\eta}\, d\theta = \int_{-\pi}^{-\epsilon} \frac{1}{g^2(\theta) + i\eta}\, d\theta + \int_{\Gamma^u_\epsilon} \frac{1}{g(\theta) + i\eta}\, d\theta + \int_{\epsilon}^{\pi} \frac{1}{g(\theta) + i\eta}\, d\theta. \tag{3.20}$$

of course we must choose the opposite path for the other integral

$$\int_{-\pi}^{\pi} \frac{1}{g(\theta) - i\eta}\, d\theta = \int_{-\pi}^{-\epsilon} \frac{1}{g(\theta) - i\eta}\, d\theta + \int_{\Gamma^d_\epsilon} \frac{1}{g(\theta) - i\eta}\, d\theta + \int_{\epsilon}^{-\pi} \frac{1}{g(\theta) + i\eta}\, d\theta. \tag{3.21}$$

Thus for any $\epsilon > 0$ we can find a suitable complex neighborhood of the origin in which both integrals on the left-hand sides of (3.20) and (3.21) are analytic functions of η since the integrands on the respective right-hand sides have no singularities along the path of integration. Therefore the function $f(\eta)$ is analytic at $\eta = 0$.

Furthermore, we obtain

$$\lim_{\eta \to 0} \int_{-\pi}^{\pi} \frac{\eta}{g^2(\theta) + \eta^2} \frac{d\theta}{2\pi} = \left(2 \frac{d^2 E_{2N+1}(\theta)}{d\theta^2} \right)^{-1/2}_{\theta = 0}. \tag{3.22}$$

By adopting a notation widely used in solid-state physics we can write the right-hand side of (3.22) as

$$(m^*_{2N+1}(0)/2)^{1/2},$$

$m^*_{2N+1}(0)$ being the so-called effective mass evaluated at the left boundary of the $(2N+1)$st band.

Now we must show the analyticity of the operator function $M^{(1)}_{E(\eta)}$ at the origin which is equivalent to showing that the function

$$(\psi, M^{(1)}_{E(\eta)} \psi) = \int_0^{2\pi} \frac{|(\psi, W^{1/2}\phi^{(\theta)}_{2N+1})|^2 - |(\psi, W^{1/2}\phi^{(0)}_{2N+1})|^2}{[E_{2N+1}(\theta) - E_{2N+1}(0)] + \eta^2} \frac{d\theta}{2\pi} \tag{3.23}$$

is analytic at $\eta = 0$ for any $\psi \in L^2(R)$. Let us show that the function

$$p(\theta) = |(\psi, W^{1/2}\phi^{(\theta)}_{2N+1})|^2 - |(\psi, W^{1/2}\phi^{(0)}_{2N+1})|^2$$

can be analytically extended to a complex neighborhood of the origin. As follows from our analysis of Sec. II, the generalized eigenfunctions of our Hamiltonian are given by the Bloch functions

$$\phi^{(\theta)}_n(x) = A^{(\theta)}_n e^{im\theta} \big[\cos\sqrt{E_n(\theta)}\,(x - 2m\pi) - ((1 - e^{i\theta})/(1 + e^{i\theta})) \cot \sqrt{E_n(\theta)}\,\pi \times \sin \sqrt{E_n(\theta)}\,(x - 2m\pi) \big], \tag{3.24}$$

for $x \in [(2m-1)\pi, (2m+1)\pi]$ and for any m.

Since the eigenfunctions (3.24) are real-analytic functions of θ it follows that

$$P(\theta) = | W^{1/2}\phi^{(\theta)}_{2N+1} \rangle \langle W^{1/2}\phi^{(\theta)}_{2N+1} |$$

is a real-analytic rank-one operator-valued function due to the fact that $W^{1/2}\phi^{(\theta)}_{2N+1}$ is a real-analytic $L^2(R)$-valued function. From (3.24) we have for θ in a small neighborhood of 0

$$|\phi^{(\theta)}_{2N+1}(x)| \leqslant 2 e^{|\Im \sqrt{E_{2N+1}(\theta)}|\pi} e^{|\Im\theta|\,|m|} \tag{3.25}$$

for any $x \in [(2m-1)\pi, (2m+1)\pi)$.

We notice that for any $|m| > 2$, $e^{|\Im\theta|\,|m|}$ is bounded by $e^{(3/2)|\Im\theta|\,|x|}$.

Therefore if $|\Im\theta| < \frac{2}{3}\alpha$ it follows from our assumption on W that $W^{1/2}\phi^{(\theta)}_{2N+1} \in L^2(R)$, which is equivalent to saying that in any neighborhood of 0 satisfying $|\Im\theta| < \frac{2}{3}\alpha$, $P(\theta)$ defined as above is an analytic rank 1 operator-valued function which implies that $p(\theta)$ has an analytic extension to a complex neighborhood of the origin. This fact allows us to use a procedure similar to the one used for the function $f(\eta)$ in order to show that the function $(\psi, M^{1)}_{E(\eta)}, \psi)$ can be analytically extended to a complex neighborhood of $\eta = 0$.

By going back to Eq. (3.17) we obtain that the left-hand side is jointly analytic in η and λ.

Furthermore we get

$$\begin{cases} F(\eta,\lambda)|_{\eta=\lambda=0} = 0, \\ \left.\dfrac{\partial F}{\partial \eta}\right|_{\lambda=0} = 1. \end{cases} \tag{3.26}$$

Thus we are allowed to apply the implicit function theorem in order to obtain the existence of the function $\eta(\lambda)$ solution of (3.17) in a complex neighborhood of 0 and its analyticity at $\lambda = 0$.

By computing the first term in the Taylor expansion of $\eta(\lambda)$ around $\lambda = 0$ we get

$$\eta(\lambda) = (m^*_{2N+1}(0)/2)^{1/2} \| W^{1/2}\phi^{(0)}_{2N+1} \|_2^2 \lambda + o(\lambda), \tag{3.27}$$

which implies

$$\eta^2(\lambda) = (m^*_{2N+1}(0)/2) \| W^{1/2}\phi^{(0)}_{2N+1} \|_2^4 \lambda^2 + o(\lambda^2) \tag{3.28}$$

and

$$\widetilde{E}_{2N+1}(\lambda) = E_{2N+1}(0) - \frac{m^*_{2N+1}(0)}{2} \times\left(\int_{-\infty}^{+\infty} |W(x)| [\phi^{(0)}_{2N+1}(x)]^2 \, dx\right)^2 \lambda^2 + o(\lambda^2).$$

In the case of a gap of the type $((N-\frac{1}{2})^2, E_{2N}(\pi))$ we have the analogous formula given in the statement of the theorem. Q.E.D.

Remark: A similar result can be shown in the case of a piecewise continuous periodic potential since also in that case the Bloch eigenfunctions can be analytically continued in a neighborhood of $\theta = 0$, if W has an exponential decay and similar formulas can be found for the bound states occurring in the gaps of the spectrum.

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