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LETTER TO THE EDITOR

Vanishing gaps in 1D bandstructures

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Abstract. The criterion for vanishing or zero-energy gaps in the spectrum of 1D electronic bandstructures is obtained from perturbation theory. It is in agreement with examples of periodic potentials which never exhibit zero-gaps as well as with those which may, including certain smooth periodic potentials. The results have relevance to recent work in the field of semiconductor layered heterostructures or superlattices. The analysis should also have implications for other problems that involve Hill's determinant.

Rigorous results for electronic energy bands exist mainly for 1D [1–3] where the general results describe energy bands varying monotonically from minimum to maximum energy from the centre of the Brillouin zone to the boundary of the first Brillouin zone, or vice versa, with gaps separating successive bands, which are infinite in number. However, the occurrence of vanishing gaps, or zero-energy gaps (ZEG), revives from time to time [4–8] and has remained an open question. While these *do not occur* in some well known models, e.g. the Mathieu problem [9], the 'Dirac comb' limit [10] of the Krönig–Penney (KP) model, nor apparently in the sawtooth (triangular wave) potential [11], they *do appear* in studies of rectangular KP models and a hybrid of triangular wells separated by flat interstial regions [5], amongst others, and so the question arises as to what are the necessary characteristics of periodic potentials for the appearance of vanishing (i.e. disappearance of) energy gaps. In recent years some of these 1D models, especially various KP models [12], but also sawtooth (triangular periodic) models for δ-doping [13], have been helpful in the topical context of semiconductor heterostructures and other superlattices [8, 14] where molecular beam epitaxy can be used to fabricate a good approximation to any desired potential profile. Of course, one does not expect the criteria for vanishing gaps in 1D to be met precisely, in the same sense that certain exotic van Hove singularities are not fully realized, but surely our results have relevance to anomalously small band gaps. Our interest in these questions was stimulated by a systematic numerical study [11] of simple periodic potentials and in this letter we present our recent analytic understanding of this question.

There are a whole set of rigorous theorems [3] which give very restrictive conditions on the narrow classes of potentials having *infinitely many* ZEGs. It follows that in some rigorous sense *almost all* periodic potentials possess open gaps, and the existence of ZEGs is the exceptional case, needing some constraints on the model parameters.

Let us note that there may be connections with other quantum problems, e.g. the search for gaps in photonic band structures [15], the anharmonic oscillator [16], as well as many others that predate quantum mechanics and electronic energy bands, since the mathematical problem of periodic perturbations goes back to Hill's equation in classical problems [17] where examples range from astronomical calculations to the inverse pendulum.

We consider the 1D operator $(-\Delta + V)$ where $V(x + 2\pi n) = V(x)$, n is any integer number, and 2π is the lattice parameter. It is shown in [3] that the edges of the gaps in the spectrum of this operator may be obtained in the following way.

Consider the operators

$H_{\mathrm{p}} = -\mathrm{d}^2/\mathrm{d}x^2 + V$ on $L^2([0, 2\pi], \mathrm{d}x)$ with periodic boundary conditions; and

$H_{\mathrm{a}} = -\mathrm{d}^2/\mathrm{d}x^2 + V$ on $L^2([0, 2\pi], \mathrm{d}x)$ with antiperiodic boundary conditions.

Let $E_1^{\mathrm{p}}, E_2^{\mathrm{p}}, ..$ be the eigenvalues of H_{p} and $E_1^{\mathrm{a}}, E_2^{\mathrm{a}}, \ldots$, correspondingly, of H_{a}, and also let

$$\alpha_n = \begin{cases} E_n^{\mathrm{p}} & n \text{ odd} \\ E_n^{\mathrm{a}} & n \text{ even} \end{cases} \qquad \beta_n = \begin{cases} E_n^{\mathrm{a}} & n \text{ odd} \\ E_n^{\mathrm{p}} & n \text{ even.} \end{cases} \tag{1}$$

Then $\cup_{n=1}^{\infty} [\beta_n, \alpha_n]$ is the set of gaps.

We have derived the criterion for the existence of ZEGs using the techniques of Malyshev and Minlos [18] for the case of the even gaps which appear at the centre of the Brillouin zone by restricting consideration to H_{p}. The procedure is similar for the odd gaps, which appear at the first Brillouin boundary, using instead H_{a}, and the derivation is the same.

It is convenient to introduce the basis $\phi_n = (2\pi)^{-1/2} \exp(\mathrm{i}nx)$. Then if ψ solves $H_{\mathrm{p}}\psi = E\psi$ and $a_n = (\phi_n, \psi)$, we find

$$(n^2 - E)a_n + \sum_{-\infty}^{\infty} V_m a_{n+m} = 0 \tag{2}$$

where $V_m = (\phi_m, V)$. This infinite determinant (Hill's) for the eigenvalues has diagonal elements $(n^2 - E)$ bordered by parallels containing successively $V_1, V_2, \ldots$ which are the Fourier coefficients of the potential [19].

All even gaps vanish in the free-electron limit, since for $V = 0$ the eigenvalues of H_{p} are n^2, $n = 0, \pm 1, \pm 2, \ldots$. These are doubly degenerate, associated with oppositely placed pairs of reciprocal lattice vectors $(\pm n)$, so that $\beta_n = \alpha_{n+1}, n = 1, 2, \ldots$, and this gives the essence of the 1D problem.

To consider the splitting of these doubly degenerate pairs for the $2n$th gap, $n = 1, 2, \ldots$, we use perturbation theory [20]. Details of the extensive remapping of the matrix will be given elsewhere [21]. If the edges are given by

$$\epsilon_{1,2} = \lambda \pm \Delta \tag{3}$$

where λ is the mean eigenvalue of the pair and Δ determines the splitting, it can be shown [21] that

$$\lambda = n^2 + \sum_{m \neq n, -n} \frac{V_{n-m}^2}{n^2 - m^2} + \mathrm{O}\left(\frac{V^3}{n^2}\right) \tag{4}$$

$$\Delta = V_{2n} + \sum_{m\neq n,-n} \frac{V_{n-m}V_{n+m}}{n^2 - m^2} + \mathrm{O}\left(\frac{V^3}{n^2}\right) \tag{5}$$

where $V \equiv ||V||_{L_1} = \sum_i |V_i|$. Thus the only condition for the $2n$th gap to vanish is

$$\Delta = 0 \tag{6}$$

which thereby is our criterion for the existence of ZEGs.

Our perturbation results are valid if the criterion for the smallness of the perturbation $||V|| \ll w$ (where $||V||$ is the norm of the potential energy operator, $||V|| \leqslant V$; w is the distance between the level considered and the set of all other points of the unperturbed spectrum, i.e. the energy difference to the next closest free-electron eigenvalues, such that $w > n$ holds). So the results are true if the inequality

$$V \ll n \tag{7}$$

holds, meaning that strictly this applies to high-lying gaps only: the energy of the gap $E_n \sim n^2 > n \gg V$ means that the energy of this gap is much higher than the top of the potential. Nevertheless we will see that in all known examples our predictions for the presence or absence of ZEGs are consistent with existing band gap knowledge.

For the odd gaps we find a splitting Δ' for the $(2n+1)$th gap, $n = 0, 1, \ldots$

$$\Delta' = V_{2n+1} + \sum_{m\neq n,-n-1} \frac{V_{n-m}V_{n+m+1}}{(n+1/2)^2 - (m+1/2)^2} + \mathrm{O}\left(\frac{V^3}{n^2}\right) \tag{8}$$

and the criterion for the $(2n+1)$th gap, $n = 0, 1, 2, \ldots$ to vanish is $\Delta' = 0$, where Δ' is defined by (8) under the same restriction (7) on the potential.

Our criterion in (6), taken with (5) and (8), may be interpreted initially as $V_n = 0$, which has some application, or as $V_n \approx 0$ with corrections supplied by the higher order terms, or in full, as will be seen in our examples below.

Let us first discuss examples with *no vanishing gaps*. It should be clear from above that our perturbation results concern high-lying gaps, and that some caution needs to be exercised in applying the results to low-lying gaps. In fact a greater generality is afforded by many of the results.

For the pure cosine potential (the Mathieu problem) [9] the high-lying gaps (for which $n > V$, where V is the top of the potential) cannot vanish. Since there is only one non-zero Fourier coefficient, V_1, the first non-zero term in the perturbation series for the nth gap is of order n

$$\Delta E \simeq \frac{V_1^n}{(2n)!} > 0 \tag{9}$$

so that high-lying ZEGs are absent in accordance with the exact result [3].

For the Dirac comb described by $V(x) = \sum_{n=-\infty}^{n=\infty} A\delta(x - 2\pi n)$, A being the strength of the δ-function, the criterion $n > V$ is not applicable but we may use perturbation theory formally if $A \ll n$ to give

$$\Delta E \sim A + \mathrm{O}(A^2/n) > 0 \tag{10}$$

in accordance with the exact result [10]. Again no gaps vanish.

Now let us consider the triangular periodic or sawtooth potential which has the Fourier series

$$V(x) = \sum_{n=1}^{\infty} V_n \cos(nx) \qquad V_n = \frac{4U}{n^2\pi^2}[(-1)^n - 1]\,. \tag{11}$$

Clearly $V_{2n} = 0$ for any n and all non-zero terms have the same sign. An accurate estimate of the second order terms gives

$$\Delta E \sim \left(\sum_{m \neq \text{odd}} \frac{1}{m^2(2n-m)^2(n^2-m^2)} \right) \frac{64U^2}{\pi^4} = C\frac{U^2}{n^3} > 0 \tag{12}$$

where $C \sim 1$, which means that high-lying even gaps are all open. For the odd gaps one finds

$$\Delta E = V_{2n+1} + \mathrm{O}\left(\frac{U^2}{n^3}\right) \sim \frac{|U|}{n^2} + \mathrm{O}\left(\frac{U^2}{n^3}\right) > 0\,. \tag{13}$$

Now we discuss examples which *do exhibit vanishing gaps*. Almost all reports of ZEGs are concerned with KP models [4, 5, 7] which are piecewise flat, except for Lin and Smit's study [5] of triangular wells separated by flat sections. One develops the impression that in some way flat sections are associated with this phenomenon. This may be dispelled by considering the truncated 3×3 matrix from (2) for the lowest three eigenvalues corresponding to reciprocal lattice vectors for $n = 0, \pm 1$ and finding its eigenvalues. This is a finite model for the following smooth potential

$$V(x) = V_1 \cos(x) + V_2 \cos(2x) \qquad V_1, V_2 \ll 1. \tag{14}$$

For small V_1, V_2 the degeneracy condition for the first even gap (the $2n$th gap for $n = 1$) occurs for

$$V_2 = -V_1^2 + \mathrm{O}(V_1^3). \tag{15}$$

For example, if $V_2 = -0.25$ we find that $V_1 = 0.559\,017\ldots$ from this approximation. A more precise value may be found numerically using larger determinants with the method described earlier [19]. In any case this is exactly the perturbation criterion of second order perturbation theory for the first even ZEG from (5) if we omit other terms of higher order. We note that Strandberg [6] has also realized that ZEGs can occur for smooth potentials in a discussion for deep wells using arguments from inverse scattering theory. However he does not give a criterion comparable with our (5), (6).

For the Krönig–Penney model a simple 'geometrical' interpretation of some ZEGs was given by Lin and Smit [5] as follows: take b for the length of the plateau, c for the length of the well, such that $(b + c) = 2\pi$, W for the depth of the wells, with $\hbar = 1$, $m = 1/2$. Then join smoothly m_1 half-wavelengths over the barrier with m_2 half-waves across the well so that $kb = m_1\pi$ and $Kc = m_2\pi$, with corresponding free-electron energies given by $E = k^2$ and $W + E = K^2$. This construction for a given E corresponds to two identical eigenvalues (degenerate) and to two linearly independent solutions [5]. The corresponding depth of the well for ZEGs follows and is

$$W = \left(\frac{m_2\pi}{2\pi - b}\right)^2 - \left(\frac{m_1\pi}{b}\right)^2 \tag{16}$$

with a threshold value b_0 when $W = 0$

$$b_0 = \frac{2\pi m_1}{m_1 + m_2}. \tag{17}$$

In applying our general analysis to the KP model we need the Fourier decomposition

$$V(x) = \sum_n \left[-\frac{W}{n\pi}\sin\left(\frac{nb}{2}\right)\right]\cos(nx). \tag{18}$$

So, according to our criterion (6), (5) and (8), the initial condition for the nth gap to be vanishing is $V_n \approx 0$, i.e. $\sin(nb/2) \approx 0$, or $nb \approx m_1 2\pi$. If we take

$$b = b_0 + \delta \qquad b_0 = 2\pi\frac{m_1}{n} \tag{19}$$

we can compare (17) and (19) to see that $n = m_1 + m_2$. Omitting details [21] we can show that

$$W = k(m_1, m_2)\delta \tag{20}$$

where $k(m_1, m_2)$ is a coefficient of order n^2 dependent on m_1 and m_2. Then since $W \ll n$, it follows that $\delta \ll n^{-1}$. From (16) and (19) we find that

$$W \approx \frac{n^3}{\pi}\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\delta + \mathrm{O}(\delta^2) \tag{21}$$

which is in agreement with (20).

In summary, following the criterion that we have developed for ZEGs, we have illustrated its value in several ways. The perturbation criterion is confirmed by application to known models without ZEGs (Mathieu, Dirac, etc) and we proved the absence of high-lying ZEGs for the triangular case. In addition to the examples presented here we have also studied a smooth potential introduced by Wille *et al* [22] which has no ZEGs, Lin and Smit's alternating constant and triangular profile [5] which may, another potential that may be described as a superposition of a KP potential and negative Dirac combs which exhibits a ZEG below the bottom of KP wells, and have found the corresponding conditions for ZEGs in other generalized KP (sectionally constant) superlattice models. Details of these calculations will be reported later [21]. These various tests show that the conditions for the existence of vanishing gaps have been established by our analysis. When the Fourier series of a periodic potential exists (is well behaved) these conditions involve special relations between those Fourier coefficients which have been obtained for high-lying gaps via a systematic perturbation approach that appears to yield quite strong results. We have also seen from our studies, supported by the discussion of the finite 3×3 approximation

[21], that *ZEGs can occur for smooth periodic potentials*, laying to rest the impression that developed through earlier KP studies, and enhanced by Lin and Smit's [5] study of the triangular well with flat plateau. Clearly there is no need for a flat plateau, nor for a discontinuity in slope between interstitial region, nor for the top of the potential to be flatter than the bottom, nor in fact for ZEGs to only appear above a plateau. Also in a separate article [23] we will present a number of numerical illustrations that may now be understood in the light of the present analysis. Some new progress can perhaps also be made with the help of the present approach in higher dimensions and it would be interesting to consider extensions for the single impurity problem. The impact on classical problems also merits further study.

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