Band structure engineering: A simple way to optimize key features of one-dimensional energy bands

David E. Rourke,* Larisa A. Khodairanova, and T. Mark Fromhold

School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, United Kingdom

(Received 22 February 2005; published 31 October 2005)

We determine the one-dimensional periodic potential required to produce an energy band structure in which the effective mass \( m^* \) at the bottom of the first miniband is minimized, and the peak group velocity within the miniband is maximized, subject to the constraint of maintaining a fixed specified energy gap \( \gamma_1 \) between the first and second bands. This problem is of considerable interest for the design of semiconductor superlattices and optical lattices that exhibit high carrier mobility combined with low interband Zener tunneling. We show that the problem is solved by a class of periodic potentials, known as 1-gap potentials, which, remarkably, support only two distinct energy bands separated by a single energy gap. We use the unique properties of 1-gap potentials to derive semi-analytical formulae that can be used to predict, \textit{ab initio}, the potential profile required to generate any physically possible value of \( m^* \) or \( \gamma_1 \). Our results provide a simple, but powerful, band structure engineering tool that should facilitate the design of superlattice structures and optical lattices with optimized transport properties.

DOI: 10.1103/PhysRevB.72.155334

PACS number(s): 73.20.At, 73.21.Cd

I. INTRODUCTION

Understanding the quantum-mechanical properties of electrons in periodic potentials is of fundamental importance in condensed matter physics. One of the first predictions of quantum theory was that periodic potentials produce allowed energy bands separated by forbidden gaps. Subsequent experimental demonstrations that energy bands control the behavior of many crystalline materials and, in particular, determine whether the material is an insulator, conductor, or semiconductor (see, for example, Ref. 1), brought rapid advances in materials technology and engineering.

For many years, experimental studies of quantum phenomena in periodic potentials could only be performed on natural three-dimensional crystals, in which a given unit cell generates a fixed energy band structure characteristic of each different material. However since the pioneering work of Esaki, Tsu, and Döhler,\textsuperscript{2,3} it has been possible to produce artificial quasi-one-dimensional crystal structures, known as superlattices (SLs), whose one-dimensional energy (mini-) band structure can be changed by altering the layer parameters. Usually, SLs are made from alternating layers of two different semiconductor materials, deposited by molecular beam epitaxy, which produce a one-dimensional periodic square potential for conduction electrons. Changing the width and composition of the wells and barriers provides some control of the energy-wave-vector \( E(k) \), dispersion relations of the minibands. For example, monolayer-thin barriers produce exceptionally wide (>100 meV) minibands, characterized by high peak electron velocities. These wide-miniband structures have greatly increased the operating frequencies of SL THz sources, in which electromagnetic radiation is produced by oscillating charge domains.\textsuperscript{4–6} However, since simple two-component SLs with square potential profiles have so few adjustable parameters, they offer only limited control of the miniband structure. More effective and flexible band structure engineering requires more complex potential profiles. For example, recent experiments\textsuperscript{7,8} used a type of GaAs/AlAs/InAs SL, in which the unit cell comprises three different materials, to obtain improved electrical performance by increasing the energy gap \( \gamma_1 \) between the first and second minibands, thereby suppressing interminiband Zener tunneling. Preventing Zener breakdown is important for limiting the current flow and power dissipation in SLs, and for ensuring that their measured electrical properties can be accurately modeled and predicted using simple single-miniband transport formalisms.

In general, it is straightforward to calculate the miniband structure corresponding to any given periodic potential. By contrast, it is much more difficult to predict the unit cell structure required to produce minibands with specified \( E(k) \) relations in which, for example, \( \gamma_1 \) is maximized. Inverse scattering methods,\textsuperscript{9} and pseudopotential calculations\textsuperscript{10} have been used to predict the three-dimensional atomic structures required to produce materials with certain optimized properties, for example the largest optical band gap. However, these calculations are difficult to perform because they involve complex optimization algorithms such as evolutionary search methods,\textsuperscript{11} and require a great deal of expertise and computer power to implement.

By contrast, in this paper we show that the potential profiles required for optimizing key parameters of one-dimensional energy bands are, in fact, easy to predict \textit{a priori} and can be expressed in simple semi-analytical formulae. We consider the particular problem of maximizing the curvature \( \left. \frac{d^2E}{dk^2} \right|_{k=0} \) of the lowest miniband at \( k=0 \), and thereby minimizing the corresponding electronic effective mass \( m^* \), while maintaining any desired fixed value of the miniband gap \( \gamma_1 \) that is physically attainable. The one-dimensional periodic potential that solves this optimization problem also maximizes the width \( \Delta \) of the lowest energy band and the peak group velocity \( v_{g,\text{max}} = \max_{0 \leq k < \pi} \left( \frac{\partial E}{\partial k} \right) \) for an electron within that band.

This problem is of considerable practical importance in SL design, where a low effective mass is essential for attain-
ing high electron mobility (a high group velocity is required in high-frequency applications\textsuperscript{6}), but a high value of $\gamma_1$ is also required to prevent Zener breakdown of the device. By considering properties of the solutions of Hill’s equation (equivalent to the Schrödinger equation for a particle in a periodic potential) that have previously been of largely mathematical interest,\textsuperscript{12} we show that $d^2E/dk^2\rvert_{k=0}$ and $v_{g,\text{max}}$ are maximized for a particular class of periodic potential, known as 1-gap potentials. The essential feature of 1-gap potentials is that, remarkably, they generate only two allowed bands separated by a single energy gap. Our analysis yields simple semi-analytical formulae that reveal a monotonic relation between the depth of the periodic potential, and the values of $d^2E/dk^2\rvert_{k=0}$ and $\gamma_1$. In particular, as the potential deepens, $\gamma_1$ and $m^*$ both increase monotonically.

Our semi-analytical formulae provide a simple tool for predicting the potential profile required to make real SL devices with specified band parameters. We hope that this will be useful to experimentalists and crystal growers requiring a straightforward way to design samples. The results of our calculations are, we believe, of broad interest because they also provide new insights for the design of other onedimensional systems for which band structure effects are of crucial importance, in particular optical lattices\textsuperscript{13–18} in which the potential energy of ultra-cold atoms varies sinusoidally with position, and photonic crystals for light (see, for example, Refs. 19 and 20). Both types of structure are being widely studied at the moment because of the interesting new physics that they reveal and their potential for technological application.

The paper is organized as follows. In Sec. II, we introduce the basic theory of one-dimensional energy bands, define 1-gap potentials, and explore their properties. In Sec. III, we consider the band structure optimization problem specified above, and prove that 1-gap potentials provide a unique solution to this problem. The key results of our analysis are presented in Sec. IV, where we use the properties of 1-gap potentials and their energy band structures to derive the semi-analytical expressions for $d^2E/dk^2\rvert_{k=0}$ and $\gamma_1$ as functions of the potential depth. In Sec. V, we compare how $d^2E/dk^2\rvert_{k=0}$ varies with $\gamma_1$ for both 1-gap potentials and sinusoidal potentials, and hence show that optical lattice potentials and band structures can, in many cases, be designed using the analytic expressions of Sec. IV. In Sec. VI, we present an example that illustrates the application of our semi-analytical formulae in an actual design problem, and confirms the validity of our predictions for 1-gap and sinusoidal potentials. Finally, in Sec. VII we present our conclusions.

In order to make our results immediately accessible to readers who may want to use them as a practical design tool, but do not want to work through the detailed analysis in Sec. III, we have tried to write Sec. IV so that it can be read independently, without first reading Sec. III. For the purpose of sample design, Eqs. (22), (24), and (29) are the key results of our paper: Eq. (22) determines the periodic potential required to maximize $d^2E/dk^2\rvert_{k=0}$ [the maximum value is given by Eq. (29)] for any desired value of $\gamma_1$ specified using Eq. (24).

FIG. 1. Typical $E$ vs $k$ curve. The lowest three allowed energy bands are shown, using an extended zone scheme. The $j$th forbidden band is at $|k|=j\pi$, and occupies the energy interval $\lambda_{2j-1}<E<\lambda_{2j}$ $(j=1,2,3,\ldots)$. It has width $\gamma_j$.

II. BACKGROUND THEORY

The Schrödinger equation\textsuperscript{21} for an electron of mass $m\textbar$ and energy $\bar{E}$ in a periodic potential $\bar{V}(X)$ with period $a$,

$$\frac{-\hbar^2}{2m} \frac{d^2\bar{\psi}}{dX^2} + \bar{V}(X)\bar{\psi} = \bar{E}\bar{\psi},$$

(1)

can be written in the dimensionless form (often called Hill’s equation\textsuperscript{22–26}),

$$\frac{d^2\bar{\psi}}{dx^2} + V(x)\bar{\psi} = E\bar{\psi},$$

(2a)

where

$$x = X/a, \quad V(x) = 2\bar{m}a^2\bar{V}(X)/\hbar^2,$$

$$E = 2\bar{m}a^2\bar{E}/\hbar^2, \quad \text{and} \quad \gamma(x) = \phi(X).$$

(2b)

Here the dimensionless potential $V(x)$ has period 1; i.e., $V(x) = V(x+1)$.

It is well known from Floquet theory (Ref. 22, Sec. 1.2) or, equivalently, from Bloch’s theorem (Ref. 1, Ch. 8), that Hill’s equation always has two solutions, $u(x)$ and $v(x)$, which satisfy

$$u(x + 1) = e^{ik}u(x)$$

(3a)

$$v(x + 1) = e^{-ik}v(x),$$

(3b)

where $u(x)$ and $v(x)$ are the Bloch wave functions.

The parameter $k$, the pseudo- (or crystal) momentum, is a function of $E$, and can be real or complex. If $k$ is real, then $|e^{ik}| = 1$, and the solutions $u(x)$ and $v(x)$ are finite-valued for all $x$, provided that they are bounded over the interval $0 \leq x < 1$. This corresponds to $E$ being in an allowed energy band. If $k$ is complex, $u(x)$ and $v(x)$ diverge as either $x \to -\infty$ or $x \to \infty$. In this case, no physically reasonable solution to Hill’s equation exists, which corresponds to $E$ being in a forbidden band, or energy gap.

Figure 1 shows the $E(k)$ curve for a typical band structure, in the extended zone scheme.\textsuperscript{27} Features of this curve that are common to all band structures include the following. There is an energy ($E=\lambda_0$, in Fig. 1) at which $k=0$, and below
which $k$ is always complex. Therefore propagating Bloch states with energies less than $\lambda_0$ are forbidden. Above $E = \lambda_0$, there is a succession of allowed and forbidden bands. The edges of the $j$th energy gap are at $|k| = j\pi$, where $j = 1, 2, 3, \ldots$. Alternatively, if $F$ is defined by

$$F = \cos k,$$

then $F = (-1)^j$ at the edges of the $j$th gap.

Let the $j$th gap occur for energies in the interval $\lambda_{2j-1} < E < \lambda_{2j}$, so that

$$\gamma_j = \lambda_{2j} - \lambda_{2j-1}$$

is the width of this gap. It is possible for a gap to have zero width. For most potentials, however, all gaps have a non-zero width, although the width of the $j$th gap tends to zero as $j \to \infty$.

Some potentials are special, however, in that the $(n+1)$th and higher gaps all have zero width. Such a potential is known as an “$n$-gap” potential. A trivial example is the potential $V(x) =$ constant, whose gaps all have zero width, and is therefore a 0-gap potential. All 1-gap potentials can be expressed in terms of Jacobi elliptic functions. They are crucially important in the band design problem of this paper, and are discussed below. Closed form expressions for 2-gap and higher potentials are not known, although they can be calculated numerically (see, for example, Ref. 26).

The quantity $F$ defined in Eq. (4) [or sometimes $\Delta = 2F$] is known as the discriminant of Hill’s equation (Ref. 22, Ch. 2). This is an entire, and hence single-valued, function of $E$ (Ref. 22, Theorem 2.2; Ref. 35). Over the $j$th allowed band, $k$ takes values in the range $(j-1)\pi < |k| < j\pi$. Let us assume that $k$ is restricted to the positive range $(j-1)\pi < k < j\pi$. Since $\cos k$ is then a monotonic function of $k$, it follows from Eq. (4) that $k$ will be a single-valued function of $F$, and of $E$.

This means that each $E$ versus $k$ curve can have no turning points in the interval $(j-1)\pi < k < j\pi$. Otherwise there would exist values of $E$ with more than one corresponding $k$ value, in contradiction to the preceding paragraph. Since $E(k)$ is an even function of $k$, there can be no turning points in the interval $(j-1)\pi < k < j\pi$, either. This means that turning points in the $E(k)$ curves for any one dimensional periodic potential can only occur at the band edges where $k = j\pi$ ($j = 0, \pm 1, \pm 2, \ldots$). Additional minima, which often occur in three-dimensional crystals, cannot be realized in one-dimensional (1D) SL systems.

III. THE BAND DESIGN PROBLEM

The band design problem is to determine the 1D periodic potential required to produce a specified band structure (in practice, several different potential profiles may generate the same band structure).

This paper principally considers the problem of finding the potential that maximizes the curvature, $d^2E/dk^2|_{k=0}$, at the center of the lowest $E$ versus $k$ curve, for a given value of the energy gap $\gamma_1 = \lambda_2 - \lambda_1$ between the lowest two allowed bands. Equivalently, the problem is to minimize the effective mass

$$m^* = 2\tilde{m}(d^2E/dk^2|_{k=0})$$

for a given band gap $\gamma_1$. [This definition of effective mass is equivalent to the usual definition $m^* = \hbar^2/(d^2E/dk^2|_{k=0})$, where $\tilde{k} = k/a$ is the pseudo-momentum for system (1) with period $a$.] Solving this problem is of great physical interest since it enables the design of SL structures with both a low effective mass, and a sufficiently high band gap to prevent interband Zener breakdown.

The main result of this section is that $m^*$ is minimized by 1-gap potentials, whose properties are considered in detail in Sec. IV.

A proof of this result can be obtained by making use of the analytic properties of $E(k)$, which we now consider. Due to the symmetry of $E(k)$, we will assume in the remainder of this paper that $k \geq 0$ (or, if $k$ is complex, that Re$(k) \geq 0$).

A. Analytic properties of $E(k)$

Although Fig. 1 only shows $E(k)$ for the allowed bands, $k$ is defined (but complex-valued) in the forbidden bands. At the start of the $j$th gap, assumed to have width greater than zero, $k = j\pi$ and $E = \lambda_{j-1}$. If $E$ is increased slightly to $\lambda_{j-1} + \delta E$, where $\delta E$ is real and positive, $k$ will acquire a small imaginary part, becoming $j\pi + i\delta y$, where $\delta y$ is real and positive. The imaginary part of $k$ increases as $E$ increases, reaching a maximum at $E = \tilde{\lambda}_j$, which is within the $j$th energy gap. Subsequent increases in $E$ will cause $k$ to move back down the imaginary axis. When $E = \lambda_{j-1}$, at the bottom of the $(j+1)$th allowed energy band, $k$ regains the (real) value $j\pi$.

A typical path taken in the complex $k$-plane as $E$ increases from $\lambda_0$ through five allowed and five forbidden bands is shown in Fig. 2. Each “height” $h_j$ is the maximum imaginary part of $k$ attained (at $E = \tilde{\lambda}_j$) as the $j$th gap is traversed. Note that in this example, $h_1 = 0$, and so $k$ never leaves the real axis as the fourth gap is traversed. This means that the fourth gap has zero width. In general, the width of the $j$th gap

\[ \text{FIG. 2. Typical path taken in the complex } k\text{-plane as } E \text{ is increased from } \lambda_0. \text{ In the } j\text{th allowed band, as } E \text{ increases from } \lambda_{j-2} \text{ to } \lambda_{j-1}, k \text{ moves along the real axis from } (j-1)\pi \text{ to } j\pi. \text{ In the } j\text{th gap, as } E \text{ increases from } \lambda_{j-1} \text{ to } \lambda_j \text{ and then to } \lambda_{j+1}, k \text{ leaves the real axis at } k = j\pi, \text{ moves in the positive imaginary direction to } j\pi + ih_j, \text{ and then back down to the real axis at } j\pi. \text{ Since the fourth gap has zero width in this example, } h_4 = 0. \text{ It is assumed throughout that Re}(k) \geq 0. \]
\[ \gamma_j = 0 \text{ if and only if } h_j = 0. \]  
(7)

According to the definition in Sec. II, an n-gap potential will have \( h_j = 0 \) for all \( j > n \).

Since, as stated in Sec. II, for any square-integrable potential over \( 0 < x < 1 \), the \( j \)th gap width tends to zero as \( j \to \infty \), the heights \( h_j \to 0 \) as \( j \to \infty \). In fact, for such potentials, the heights satisfy the stronger condition\(^{38,39}\)

\[ \sum_{j=1}^{\infty} j^2 h_j^2 < \infty. \]  
(8)

Remarkably, it can be shown\(^{38,39,41}\) that if the heights \( h_j \) are known, then, assuming that they satisfy inequality (8), there is a unique corresponding energy band structure and \( E(k) \) curve in an extended zone scheme (specified to within a constant shift in \( E \)). In other words, the band structure is determined completely by the heights \( h_j \), and the ground state energy \( \lambda_0 \).

If one of the \( h_j \) values is changed by a small amount (and \( \lambda_0 \) is kept constant), the \( E(k) \) curve will, in general, change. There is a very simple expression for the rate at which \( E \) changes with \( h_j \), at a fixed \( k \) value:\(^{40}\)

\[ \frac{\partial E}{\partial h_j} = \frac{\mu_j}{\tilde{\lambda}_j - \lambda_0} E - \lambda_0, \]  
(9a)

where

\[ \mu_j = \begin{cases} 
\frac{1}{d^2k/dE^2|_{E=\lambda_j}} & \text{for } h_j > 0, \\
0 & \text{for } h_j = 0.
\end{cases} \]  
(9b)

As discussed above, if \( h_j > 0 \), then at \( E=\tilde{\lambda}_j \), the imaginary part of \( k \) has a local maximum value, and in a finite neighborhood about \( \tilde{\lambda}_j \), the real part of \( k \) is constant. Therefore, \( d^2(k(i))/dE^2|_{E=\lambda_j} \) is real, and in the range \( -\infty < d^2(k(i))/dE^2|_{E=\lambda_j} < 0 \). Hence, from Eq. (9b), \( 0 < \mu_j < \infty \) if \( h_j > 0 \). Conversely,

\[ \mu_j = 0 \text{ if and only if } h_j = 0. \]  
(10)

Equation (9a) is the key to proving that 1-gap potentials solve the band design problem stated earlier.\(^{42}\)

### B. 1-gap potentials as solutions to the band design problem

Let us consider the set of \( E \) values at the band edges, \( \{\lambda_n, n=0,1,2,\ldots\} \) (see Fig. 1). At discrete wave numbers \( k=j\pi \) (\( j=1,2,\ldots \)) there are two band edge energies: \( \lambda_{2j-1} \) and \( \lambda_{2j} \). An infinitesimal change in an \( h_j \) value will change all the \( \lambda_n \) values, for \( n > 0 \), but does not change the corresponding values of \( k \). Conveniently Eq. (9a) can be used directly to find the rate at which \( \lambda_n \) changes with \( h_j \). This is simply

\[ \frac{\partial \lambda_n}{\partial h_j} = \frac{\mu_j}{\tilde{\lambda}_j - \lambda_0} \lambda_n - \lambda_0. \]  
(11)

From Eqs. (5) and (11), the gap widths, \( \gamma_n \), change as

\[ \frac{\partial \gamma_n}{\partial h_j} = -\mu_j \gamma_n \frac{1}{(\tilde{\lambda}_j - \lambda_{2n-1})(\tilde{\lambda}_j - \lambda_{2n})}. \]  
(12)

The sign of \( \partial \gamma_n/\partial h_j \) is important. If \( j \neq n, \lambda_{2n-1} \) and \( \lambda_{2n} \) are either both greater than or both less than \( \lambda_j \). Consequently, \( \partial \gamma_n/\partial h_j < 0 \), unless either \( \mu_j = 0 \) [i.e., from Eq. (10), \( h_j = 0 \)] or \( \gamma_n = 0 \) (i.e., \( n = 0 \)), in which case \( \partial \gamma_n/\partial h_j = 0 \).

If \( j=n \), Eq. (12) becomes

\[ \frac{\partial \gamma_j}{\partial h_j} = -\mu_j \gamma_j \frac{1}{(\tilde{\lambda}_j - \lambda_{2j-1})(\tilde{\lambda}_j - \lambda_{2j})}. \]  
(13)

If \( h_j > 0, \lambda_{2j-1} < \tilde{\lambda}_j < \lambda_{2j} \) and therefore \( \partial \gamma_j/\partial h_j > 0 \). If \( h_j = 0, \mu_j = 0 \) and \( \lambda_{2j-1} = \lambda_{2j} = \tilde{\lambda}_j \), and therefore the right hand side of Eq. (13) is undefined. However, by considering the limit \( h_j \to 0 \), it can be shown that\(^{40}\)

\[ \frac{\partial \gamma_j}{\partial h_j} = \frac{dE}{dk} \bigg|_{k=\pi j} \quad \text{if } h_j = 0, \]  
(14)

and this is finite and greater than zero.

Therefore, to summarize the above results,

\[ \frac{\partial \gamma_n}{\partial h_j} < 0 \quad \text{if } j \neq n \text{ and } h_j \neq 0, \]  
(15a)

\[ = 0 \quad \text{if } j \neq n \text{ and } h_j = 0, \]  
(15b)

\[ > 0 \quad \text{if } j = n. \]  
(15c)

Physically, Eqs. (15) mean that if a change in \( V(x) \) increases a single height \( h_j \) by a small amount, it also [Eq. (15c)] increases the corresponding energy gap \( \gamma_j \). Such a change decreases all of the other energy gaps [Eq. (15a)], unless [Eq. (15b)] an energy gap is already zero, or if \( h_j \) is being increased from zero. These qualitative statements can also be derived by arguments involving harmonic measure,\(^{41}\) or, equivalently, the principle of increasing flux.\(^{43,44}\)

Since \( E=\lambda_0 \) is a minimum in the lowest \( E(k) \) curve, this curve has the form, in the neighborhood of \( k=0 \),

\[ E(k) = \lambda_0 + \frac{1}{2} E''(0) k^2, \]  
(16)

to second order in \( k \), where \( E''(0) = d^2E/dk^2|_{k=0} > 0 \). If an \( h_j \) value is changed by \( dh_j \), then the \( E(k) \) curve becomes \( \hat{E}(k) \), where

\[ \hat{E}(k) = E(k) + \frac{\partial E}{\partial h_j} dh_j = E(k) + \frac{\mu_j}{\lambda_j - \lambda_0} E(k) - \lambda_0 \]  

\[ = \lambda_0 + \frac{1}{2} E''(0) k^2 + \frac{\mu_j}{\lambda_j - \lambda_0} \]  

\[ = \lambda_0 + \frac{1}{2} E''(0) k^2 \left[ 1 - \frac{\mu_j dh_j}{(\lambda_j - \lambda_0)^2} \right]^2. \]  
(17)
where Eqs. (9a) and (16) have been used, and only terms up to second order in \( k \) have been kept.

Therefore, the \( \hat{E}(k) \) curve still has a minimum at \( k=0 \), but the curvature has been changed by \( dE^n(0)=[\partial E^n(0)/\partial h_j]dh_j \), where

\[
\frac{\partial E^n(0)}{\partial h_j} = -\frac{\mu_j E^n(0)}{(\lambda_j - \lambda_0)^2},
\]

(18)

which is negative if \( \mu_j > 0 \) or, equivalently, \( h_j > 0 \) [see Eq. (10)].

Therefore, if any \( h_j > 0 \) is increased, the curvature of the lowest \( E(k) \) curve, \( d^2E/dk^2|_{k=0} \), will decrease, thus raising \( m^* \).

Given any initial set of heights \( h_j \), Eqs. (15) and (18) provide a recipe for increasing the curvature \( d^2E/dk^2|_{k=0} \) to a maximum while maintaining the lowest energy gap, \( \gamma_1 = \lambda_2 - \lambda_1 \).

Assuming initially that \( \gamma_1 > 0 \), i.e., from Eq. (7), \( h_1 > 0 \), the procedure works as follows.

1. Take any nonzero height \( h_1 (l > 1) \) and increase it by a small amount. It follows from Eqs. (15a) and (15b) that this will weakly increase (i.e., increase or keep the same) all the \( \gamma_n \) values for which \( n \neq l \).

2. Since it is assumed that \( h_1 > 0 \), it follows from Eq. (15a) that \( \gamma_1 \) will strictly increase; i.e., the first energy gap will increase in width. We must compensate for this by decreasing \( h_1 \) sufficiently for \( \gamma_1 \) to return to its initial value (the final value of \( h_1 \) will be greater than zero). This is always possible because \( \gamma_1 \) decreases continuously and monotonically as \( h_1 \) decreases [Eq. (15c)], but if \( h_1 \) reaches zero, \( \gamma_1 \) will equal zero [Eq. (7)], and so there must have been a point earlier where \( \gamma_1 \) had the correct value.

3. Steps 1 and 2 above decrease both \( h_l \) and \( h_1 \). It follows from Eq. (18) that this increases the curvature at \( E = \lambda_0 \). Repeat steps 1 and 2 until \( h_l = 0 \) (\( h_1 \) can never reach zero from the argument used at the end of step 2).

4. Finally, to maximize \( d^2E/dk^2|_{k=0} \), repeat steps 1-3 for all the nonzero heights \( h_i, l > 1 \), so that the only nonzero height remaining is \( h_1 \); i.e., the corresponding potential is a 1-gap potential.

The band structure corresponding to this 1-gap potential will have the same lowest band gap \( \gamma_1 \) as the original band structure, but its curvature \( d^2E/dk^2|_{k=0} \) must be greater. Therefore, given any potential with more than one nonzero gap width, there is always a 1-gap potential with the same lowest band gap \( \gamma_1 \), and a greater curvature. As shown in Sec. IV, 1-gap potentials are uniquely determined by \( \gamma_1 \) (up to a constant shift in \( x \) or energy). This 1-gap potential is therefore the unique potential with the greatest curvature for a given gap width \( \gamma_1 > 0 \).

Appendix A supplements this discussion by obtaining an upper limit on the decrease in \( h_l \) that is required to match any small decrease in \( h_1 (l > 1) \), given that \( \gamma_1 \) is to remain constant. In this appendix, it is confirmed that \( h_1 \) always remains positive, even in the limit of an infinite number of \( h_i \) values being decreased to zero.

Finally, note that if \( \gamma_1 = 0 \) (i.e., \( h_1 = 0 \)), then the maximum curvature is still obtained by decreasing all the \( h_i \) values \( l > 1 \) to zero, but now keeping \( h_1 = 0 \). The final potential is then a 0-gap potential, i.e., \( V(x) = \text{constant} \), which can be considered a special case of a 1-gap potential.

C. Others parameters maximized by 1-gap potentials

Our analysis can be used to show that 1-gap potentials also maximize other key parameters, for a given band gap \( \gamma_1 \). Any parameter \( p \) such that, for all \( j \geq 1 \),

\[
\frac{\partial p}{\partial h_j} < 0 \quad \text{for} \quad h_j > 0
\]

(19)

will be maximized. Examples include (i) the band width \( \Delta = \lambda_1 - \lambda_0 \), where

\[
\frac{\partial \Delta}{\partial h_j} = -\frac{\mu_j (\lambda_1 - \lambda_0)}{(\lambda_j - \lambda_0)(\lambda_j - \lambda_1)},
\]

(20)

and (ii) the group velocity \( v_g = dE/dk \), where

\[
\frac{\partial v_g}{\partial h_j} = -\frac{\mu_j v_g}{(E - \lambda_j)^2}.
\]

(21)

The right-hand side of Eq. (21) is negative if \( v_g > 0 \) and if \( h_j > 0 \). It is then straightforward to show that the peak group velocity in the first allowed band, \( v_{g,\text{max}} = \max_{0 \leq k \leq \pi}(v_g) \), is maximized by a 1-gap potential.

IV. 1-GAP POTENTIALS

The principal result of this paper, derived in the previous section, is that the maximum curvature at the bottom of the lowest \( E \) versus \( k \) curve, for a given energy gap \( \gamma_1 \) between the lowest two allowed bands, is generated by a 1-gap potential.

It is well known\(^{31-33}\) that 1-gap potentials are elliptic functions. They have the form\(^{45}\), up to an additive constant or a shift in \( x \),

\[
V_m(x) = 4mK^2(m)[2sn^2(2K(m)x|m|) - 1],
\]

(22)

where \( sn(u|m|) \) is a Jacobi elliptic function (Ref. 46, Ch. 16) and \( K(m) \) is a complete elliptic integral of the first kind (Ref. 46, Sec. 17.3.1). The parameter \( m \) can take values \( 0 < m < 1 \), although when \( m=0 \), the potential is identically zero.\(^{47}\)

For potentials of the form given by Eq. (22), Hill’s equation is also known as the Lamé equation (Ref. 48; Ref. 49, Ch. 23) for which the energies at the first three band edges are\(^{50}\)

\[
\lambda_0 = 0, \quad \lambda_1 = 4(1 - m)K^2(m), \quad \lambda_2 = 4K^2(m).
\]

(23)

It follows that the lowest (and only nonzero) gap width is

\[
\gamma_1 = \lambda_2 - \lambda_1 = 4mK^2(m).
\]

(24)

An explicit expression can be derived for the curvature, \( d^2E/dk^2 \) at \( E = \lambda_0 \), produced by the 1-gap potential [Eq. (22)].

Firstly,\(^{24}\)

\[155334-5\]
of Ref. 46, Chs. 16–17. Other notations exist, involving, for a 1-gap potential, the product only includes the roots must be chosen to ensure that $k$ travels along the path indicated in Fig. 2 as $E$ is increased. Then,

$$\frac{dE}{dk} = \frac{1}{2 \sqrt{E-\lambda_0}} \prod_{j=1}^{1} \frac{E-K_j}{\sqrt{(E-\lambda_{2j-1})(E-\lambda_{2j})}},$$ (25)

where the prime indicates that the product is taken over only those values of $j$ for which $\gamma_j > 0$. The signs of the square roots must be chosen to ensure that $k$ travels along the path indicated in Fig. 2 as $E$ is increased. Then,

$$\frac{d^2E}{dk^2} \bigg|_{k=0} = 2 \prod_{j=1}^{1} \frac{\lambda_{2j-1}-\lambda_0}{(\lambda_j-\lambda_0)^2}. \quad (26)$$

This expression is true for all periodic potentials. For a 1-gap potential, the product only includes the $j=1$ term, and hence

$$\frac{d^2E}{dk^2} \bigg|_{k=0} = 2(\lambda_1-\lambda_0)\frac{E}{(\lambda_1-\lambda_0)^2}. \quad (27)$$

However, $\tilde{\lambda}_1$ equals\(^5^0\)

$$\tilde{\lambda}_1 = 4E(m)K(m), \quad (28)$$

where $E(m)$ is the complete elliptic integral of the second kind (Ref. 46, Sec. 17.3.3-4). Therefore, from Eqs. (23), (28), and (27),

$$\frac{d^2E}{dk^2} \bigg|_{k=0} = 2(1-m)K^2(m)/E^2(m) \quad (29)$$

for a 1-gap potential.

In this section, we have expressed the elliptic functions and integrals in terms of the parameter $m$, using the notation of Ref. 46, Chs. 16–17. Other notations exist, involving, for example, the modulus $k$ or modular angle $\alpha$ rather than $m$. Algebraic packages such as MATHEMATICA\(^5^1\) and MAPLE\(^5^2\) use different notations. To clarify these differences, code is provided in Appendix B, to calculate some of the above quantities using both MATHEMATICA and MAPLE.

Figure 3 shows 1-gap potentials $V_m(x)$ for four choices of $m$. For $m=0$, $V_m(x)=0$ for all $x$, which corresponds to the free electron limit with $\gamma_1 = 0$ [see also Eq. (24) with $m=0$]. As $m$ increases, $\gamma_1$ increases monotonically, as shown in Fig. 4. From the behavior of $K(m)$ as $m \to 1$ (Ref. 46, Sec. 17.3.26), it can be shown that

$$\gamma_1 \to \log^2 \frac{1-m}{16} \quad \text{as} \quad m \to 1,$$ (30)

and therefore $\gamma_1$ increases to infinity as $m \to 1$. Any value of $\gamma_1$ in the range $0 \leq \gamma_1 < \infty$ has a unique corresponding value of $m$ in the range $0 < m < 1$, and therefore a unique 1-gap potential $V_m(x)$, up to a constant shift in $x$ or energy.

It can be shown (Ref. 46, Ch. 16) that the maximum and minimum values of the 1-gap potential are

$$V_{\text{min}} = V(x=0) = -4mK^2(m) = -\gamma_1,$$ $\quad V_{\text{max}} = V(x=\frac{1}{2}) = 4mK^2(m) = \gamma_1,$ (31)

and therefore these become infinite as $m \to 1$. This behavior is expected from a tight-binding picture, in which the energy bands originate from quantum-mechanical coupling of the discrete energy levels of each well in the periodic potential. Deeper wells have more widely spaced energy levels, corresponding to a larger value of $\gamma_1$. Energy levels in adjacent wells are more weakly coupled so that the energy bands are narrower and the effective mass is higher. Hence, the curvature $d^2E/dk^2|_{k=0}$ will be lower, as we now demonstrate.

The solid line in Fig. 5 shows how the curvature $d^2E/dk^2|_{k=0}$ varies with $m$. The maximum curvature occurs for $m=0$ (i.e., in the free-electron limit with $\gamma_1 = 0$). Equivalently, the curvature can be plotted as a function of $\gamma_1$ (see the dashed line in Fig. 5). It is clear from this figure that a compromise is needed in order to maximize both the curvature and the energy gap, $\gamma_1$, thereby combining a low effec-

![Figure 3](https://example.com/figure3.png)

**Fig. 3.** 1-gap potentials, defined in Eq. (22), for different choices of the parameter $m$. The potentials are periodic with period 1.

![Figure 4](https://example.com/figure4.png)

**Fig. 4.** Gap width $\gamma_1$ vs $m$ for 1-gap potentials [from Eq. (24)].

$$\gamma_1 \to \log^2 \frac{1-m}{16} \quad \text{as} \quad m \to 1,$$ (30)

and therefore $\gamma_1$ increases to infinity as $m \to 1$. Any value of $\gamma_1$ in the range $0 \leq \gamma_1 < \infty$ has a unique corresponding value of $m$ in the range $0 < m < 1$, and therefore a unique 1-gap potential $V_m(x)$, up to a constant shift in $x$ or energy.

It can be shown (Ref. 46, Ch. 16) that the maximum and minimum values of the 1-gap potential are

$$V_{\text{min}} = V(x=0) = -4mK^2(m) = -\gamma_1,$$ $\quad V_{\text{max}} = V(x=\frac{1}{2}) = 4mK^2(m) = \gamma_1,$ (31)

and therefore these become infinite as $m \to 1$. This behavior is expected from a tight-binding picture, in which the energy bands originate from quantum-mechanical coupling of the discrete energy levels of each well in the periodic potential. Deeper wells have more widely spaced energy levels, corresponding to a larger value of $\gamma_1$. Energy levels in adjacent wells are more weakly coupled so that the energy bands are narrower and the effective mass is higher. Hence, the curvature $d^2E/dk^2|_{k=0}$ will be lower, as we now demonstrate.

The solid line in Fig. 5 shows how the curvature $d^2E/dk^2|_{k=0}$ varies with $m$. The maximum curvature occurs for $m=0$ (i.e., in the free-electron limit with $\gamma_1 = 0$). Equivalently, the curvature can be plotted as a function of $\gamma_1$ (see the dashed line in Fig. 5). It is clear from this figure that a compromise is needed in order to maximize both the curvature and the energy gap, $\gamma_1$, thereby combining a low effec-

![Figure 5](https://example.com/figure5.png)

**Fig. 5.** Curvature, $d^2E/dk^2|_{k=0}$, at the bottom of the lowest energy band, plotted against $m$ (solid curve) and $\gamma_1$ (dashed curve), for 1-gap potentials [from Eq. (29)].
tive mass with small interband Zener tunneling rates.

There seems to be no simple expression for the maximum group velocity in the first energy band. However, the group velocity for a 1-gap potential is, from Eq. (25),

$$\frac{dE}{dk} = \frac{2\sqrt{E(\lambda_1 - E)(\lambda_2 - E)}}{(\lambda_1 - \lambda_2)}$$

(32)

for $0 \leq k \leq \pi$. It is then straightforward to find numerically $v_{g,max}$, the maximum of $dE/dk$ in the first allowed band.

Figure 6 shows the variation of $v_{g,max}$ with $m$ (solid curve) and with $\gamma_1$ (dashed curve). As for $d^2E/dk^2|_{k=0}$, a compromise would be needed to maximize both $v_{g,max}$ and $\gamma_1$.

V. OPTICAL LATTICES AND SINUSOIDAL POTENTIALS

It is apparent from Fig. 3 that 1-gap potentials have shapes similar to sinusoidal potentials, that describe the interaction between ultracold alkali atoms and a 1D optical lattice formed from two counter-propagating laser beams. The relationship between gap width $\gamma_1$ and curvature $d^2E/dk^2|_{k=0}$ shown in Fig. 5 for 1-gap potentials is therefore likely to be approximately correct for sinusoidal potentials, and might therefore provide a useful tool for the design of optical lattices, where low effective masses and Zener tunneling rates are also desirable. To explore this possibility, we first consider Hill’s equation (2a) for the period-1 sinusoidal potential $V(x) = V_0 \cos 2\pi x$. This can be written as Mathieu’s equation,

$$\frac{d^2y}{dz^2} + (a - 2q \cos 2z)y = 0,$$

(33)

where $z = \pi(x - \frac{1}{4})$, $a = E/\pi^2$, and $q = V_0/(2\pi^2)$.

The first gap width is

$$\gamma_1 = \pi^2(a_1 - b_1),$$

(34)

where $a_1$ and $b_1$ are characteristic values for the Mathieu equation (Ref. 46, Sec. 20.2). Moreover, the curvature is given by

$$\left.\frac{d^2E}{dk^2}\right|_{k=0} = \left.\frac{d^2a}{dv^2}\right|_{v=0},$$

(35)

where $v$ is the characteristic exponent of Mathieu’s equation (Ref. 46, Sec. 20.3).

Simple semi-analytical expressions for $\gamma_1$ and $d^2E/dk^2|_{k=0}$ do not exist for this potential, although they can be calculated numerically. As for the 1-gap potential, the curvature $d^2E/dk^2|_{k=0}$ is a single-valued function of gap width $\gamma_1$, shown by the solid curve in Fig. 7. This variation of curvature with $\gamma_1$ is very similar to the corresponding curve (dashed in Fig. 7) for 1-gap potentials, for a wide range of $\gamma_1$ values. This confirms that the semi-analytical formulae given in Eqs. (22), (24), and (29) can indeed be used to make fast and accurate predictions of the energy band structures corresponding to a wide range of optical lattices, and so optimize their parameters for transport studies.

In Appendix C, we show analytically that the absolute difference between the $d^2E/dk^2|_{k=0}$ values for 1-gap and sinusoidal potentials is very small in the regimes of small and large $\gamma_1$ values.

VI. EXAMPLE

To illustrate the application of the analytical expressions Eqs. (22), (24), and (29), we used them to determine the form of the 1-gap potential required to give an arbitrarily chosen fixed energy gap of $\gamma_1 = 20$ (see Appendix B for details). From Eq. (24), the value of parameter $m$ required to produce this band gap is $m = 0.858$, for which, from Eq. (29), the corresponding curvature is $d^2E/dk^2|_{k=0} = 1.28$. The 1-gap potential for this $m$ value is shown by the solid curve in Fig. 8.

To confirm this analysis and the predictions of Eqs. (24) and (29), we calculated numerically the band structure for

FIG. 7. Solid curve: curvature, $d^2E/dk^2|_{k=0}$, at the bottom of the lowest energy band, plotted against lowest gap width $\gamma_1$ for a sinusoidal potential $V_0 \cos 2\pi x$. Dashed curve: corresponding curve for 1-gap potentials.

FIG. 8. Solid line: the 1-gap periodic potential that produces an energy gap $\gamma_1 = 20$. Dots: the sinusoidal potential with the same maximum and minimum values as the 1-gap potential ($V_0 = 20$).
the 1-gap potential. The solid curve in Fig. 9(a) shows the $E$ versus $k$ curve for the lowest band, compared to that for a free electron (dashed line) with the same maximum and minimum values as the 1-gap potential (i.e., $V_{0}=20$). The $E$ versus $k$ curves calculated for this sinusoidal potential are shown by the dots in Figs. 9(a) and 9(b). The energy gap for the sinusoidal potential is $\gamma_{1} = 19.69$ and the curvature is $d^{2}E/dk^{2}{|_{k=0}} = 1.29$. It is clear from Fig. 9 that the band structure for the sinusoidal potential is very close to that of the corresponding 1-gap potential (solid curve in Fig. 8). More generally, we find that for all $\gamma_{1} = 30$, the band structures of 1-gap potentials are very similar to those of sinusoidal potentials with the same well depths, which confirms the applicability of Eqs. (24) and (29) in the design and optimization of optical lattice energy bands.

VII. CONCLUSION

We have shown that 1-gap potentials, $V_{m}(x)$, maximize $d^{2}E/dk^{2}{|_{k=0}}$, and equivalently minimize $m^{*}$, for a particle in a 1D periodic potential subject to the constraint that $\gamma_{1}$ has any specified fixed value. In practice, as in Ref. 55, such potentials could be realized in GaAs/(Al,Ga)As SL heterostructures by making the Al fraction, $f$, a continuous function of $x$ so that the local conduction band offset, given approximately by $f(x)\tilde{E}_{1}$, equals $(h^{2}/2\tilde{m}a^{2})V_{m}(x)+\tilde{E}_{1}/2$.

For GaAs/(AlGa)As structures, the maximum depth of such a potential equals the conduction band offset $\tilde{E}_{1} = 1.2$ eV of a GaAs/AlAs interface. With an effective mass in the absence of the SL potential of $\tilde{m} = 0.067m_{e}$ ($m_{e} = 9.1 \times 10^{-31}$ kg), and a SL potential of period $a = 0.436 \times 10^{-8}$ m, this corresponds [Eq. (2b)] to a dimensionless potential depth, $V_{\text{max}} - V_{\text{min}} = 40$. A 1-gap potential with this depth and period would, from Eq. (31), give a gap width of $\gamma_{1} = 20$, as in the example of Sec. VI. The effective mass at $k=0$ would then equal $2\tilde{m}/(d^{2}E/dk^{2}{|_{k=0}}) = 1.563\tilde{m} = 0.105m_{e}$.

For high-frequency applications, the maximum group velocity in the first energy band ($v_{g,\text{max}}$) is important. The same method used to optimize $m^{*}$ can also be used to optimize $v_{g,\text{max}}$; again, 1-gap potentials have the greatest $v_{g,\text{max}}$ for a given $\gamma_{1}$.

It can be seen from Fig. 3 that 1-gap potentials vary almost sinusoidally with $x$, just like optical lattice potentials for ultracold atoms in a laser standing wave. Consequently, our results for 1-gap potentials can be applied directly to the design of optical lattices. Just as for SLs, it is important to maximize the gap between the first and second energy bands of optical lattices in order to prevent Zener breakdown, which strongly suppresses semiclassical energy band transport processes such as Bloch oscillations. Since Eqs. (22) and (24) provide simple formulae for predicting the potential depth required to produce any desired value of $\gamma_{1}$, they should facilitate the design of optical lattices with the low interband tunneling rates required for the study of single-band semiclassical transport processes.

By providing a simple, easy-to-implement rule for maximizing the band curvature, while maintaining a fixed value of $\gamma_{1}$, our calculations could greatly increase the power and scope of band structure engineering as a tool for the design of next-generation SL devices, photonic structures, and optical lattices. We hope that our results will now stimulate the design of new structures that confirm the results of our calculations and offer improved transport characteristics.

ACKNOWLEDGMENTS

We thank Dr Amalia Patanè for helpful discussions. This work is supported by EPSRC.

APPENDIX A: UPPER LIMIT ON CHANGE IN HEIGHT $h_{1}$ WHEN OTHER HEIGHTS ARE CHANGED

This Appendix considers the change in the height $h_{1}$ needed when a positive height $h_{m}$ ($m > 1$) is decreased, such that the first energy gap $\gamma_{1}$ does not change. Assuming that
h_m > 0 initially, it shows that h_m will remain positive as h_m is decreased to zero. This remains true even if an infinite number of h_m values (i.e., all m > 1) are decreased to zero.

Furthermore, since dh_m is made to h_m, together with a change dh_1. If \( \gamma_1 \) is to remain constant, the condition

\[
\frac{\partial \gamma_1}{\partial h_1} + \frac{\partial \gamma_1}{\partial h_m} dh_m = 0,
\]

must be satisfied. Therefore [Eq. (12)],

\[
-dh_1 = \mu_m \frac{\lambda_1 - \lambda_1}{(\lambda_m - \lambda_1)(\lambda_m - \lambda_2)} (-dh_m).
\]

Since dh_m < 0, then dh_1 < 0, as all the terms on the right-hand side of Eq. (A2) are positive.

It is convenient to define

\[
z = \sqrt{E - \lambda_0}
\]

with corresponding quantities (chosen positive for \( j > 0 \))

\[
z_j = \sqrt{\lambda_j - \lambda_0} \quad \text{and} \quad \bar{z}_j = \sqrt{\lambda_j - \lambda_0}.
\]

Additionally, let

\[
\nu_j = \begin{cases} 
\frac{1}{|d^2k/dz|^2}_{z \rightarrow z_j} & \text{for } h_j > 0, \\
0 & \text{for } h_j = 0.
\end{cases}
\]

It can then be shown that

\[
\mu_j = 4z_j^2 \nu_j.
\]

It is also known that

\[
\nu_j = h_j.
\]

Let \( \sigma_n = z_{2n-1} - z_{2n-2} \); i.e., the change in z across the \( n \)th allowed band. Let

\[
s = \min \sigma_n,
\]

i.e., the least value of \( \sigma_n, n = 1, 2, \ldots \). It is known that

\[
s > 0,
\]

\[
\bar{z}_m - z_1 \geq \bar{z}_m - z_2 \geq s(m - 1).
\]

Therefore [Eqs. (A2), (A5), and (A3b)],

\[
-dh_1 = \nu_m \frac{z_m^2}{z_1^2} \left( \frac{z_m^2 - z_1^2}{z_m^2 - z_2^2} \right) (-dh_m)
\]

\[
= q_1 \frac{z_m^2}{(z_m - z_1)(z_m - z_2)} (z_m^2 + z_1)(z_m^2 + z_2) (-dh_m),
\]

where

\[
q_1 = \frac{1}{\nu_1} \left( \frac{z_1^2}{z_2^2} - \frac{z_1^2}{z_1^2} \right).
\]

Furthermore, since \( z_1, z_2, \bar{z}_m \) are positive,
shown that by the initial value of $z$ greater than 0. If all the

$\text{ROURKE, KHODARINOV A, AND FROMHOLD PHYSICAL REVIEW B}$

Let $h$ change such that

$$q_1 = \frac{2}{z_1} \sqrt{(\bar{z}_1 - z_1)(z_2 - \bar{z}_1)f(\bar{z}_1).}$$

(A20)

However,

$$q_1 = \frac{2}{z_1} \sqrt{(\bar{z}_1 - z_1)(z_2 - \bar{z}_1)f(\bar{z}_1).}$$

(A21)

so that

$$q_1 = \frac{2}{z_1} \sqrt{(\bar{z}_1 - z_1)(z_2 - \bar{z}_1)f(\bar{z}_1).}$$

(A22)

However since $z_1 \leq \bar{z}_1 \leq z_2$,

$$q_1 \leq 2h_1 \sqrt{2(1 + \frac{z_2}{z_1})}.$$

(A23)

so that,

$$q_1 \leq 2h_1 \sqrt{2(1 + \frac{z_2}{z_1})}.$$

(A24)

It is well known that $z_1 \leq \pi$, with equality only for a constant potential. Therefore, $s \leq z_1 \leq \pi$. Since $z_2 = z_1 + l_1$ and $l_1 \leq 2h_1$, then $z_3 = \pi + 2h_1$. Therefore,

$$q_1 \leq 2h_1 \sqrt{2(1 + \frac{z_2}{z_1})}.$$ $f_{\text{max}}$.

(A25)

Let $h_1^{(0)}$ be the value of $h_1$ before any changes to the heights were made. Then $h_j \leq h_1^{(0)}$. Similarly, let $s_j^{(0)}$ be the initial value of $s$, and $f_{\text{max}}^{(0)}$ the initial value of $f_{\text{max}}$. It can be shown that $s \geq s_0$, and therefore that $f_{\text{max}} \leq f_{\text{max}}^{(0)}$. Hence,

$$q_1 \leq s^{(0)^2} C^{(0)} h_1.$$ $h_1^{(0)}$,

(A26a)

where

$$C^{(0)} = \frac{2}{s^{(0)^2}} \sqrt{2(1 + \frac{\pi + 2h_1^{(0)}}{s^{(0)^2}}) f_{\text{max}}^{(0)},}$$

(A26b)

and $0 < C^{(0)} < \infty$.

This upper bound on $q_1$ can be used to find an upper bound on $-\Delta h_1$ in Eq. (A12):

$$-\Delta h_1 \leq \frac{C^{(0)}}{m-1} h_1 h_m (-\Delta h_m).$$

(A27)

Therefore, if $h_m$ is decreased to zero, log $h_1$ will change by $\Delta \log h_1$, such that

$$-\Delta \log h_1 \leq \frac{C^{(0)}}{2(m-1)^2} h_m^2,$$

(A28)

i.e., log $h_1$ remains finite, and therefore $h_1$ will remain greater than 0. If all the $h_m$ ($m > 1$) are decreased to zero, log $h_1$ will change such that

$$-\Delta \log h_1 \leq \frac{C^{(0)}}{2(m-1)^2} h_m^2,$$

(A29)

which is finite, by assumption (8), and hence $h_1$ remains greater than zero.

**APPENDIX B: CALCULATION OF 1-GAP POTENTIALS TO MAXIMIZE THE CURVATURE FOR A GIVEN (LOWEST) GAP WIDTH**

This Appendix gives the code needed to calculate and plot the 1-gap potential of Eq. (22) that has a gap width $\gamma_1 = 20$. The corresponding curvature [Eq. (29)] is also calculated. Finally, code to calculate and plot the discriminant $F(E)$ is given [Eq. (4)].

Code is presented using both MATHEMATICA and MAPLE code, partly to illustrate the variety of notations that different references and mathematical packages use for calculating elliptic functions. In particular, MAPLE generally expresses the elliptic functions in terms of the modulus, $k$, whereas MATHEMATICA uses the parameter $m$ (Ref. 46, Sec. 17.2.1). In both, $\lambda$ is used instead of $E$ to denote dimensionless energy.

1. MATHEMATICA (v5) code

```math
Eg = 20
m = m/. FindRoot[4*m*EllipticK[m]^2 == Eg, {m, 0.5}]
K = EllipticK[m]
V = 4*m*K^2*(2*JacobiSN[2*K*x, m]^2 - 1)
Plot[V, {x, 0, 1}]
```

2. MAPLE (v7) code

```maple
Eg := 20;
k := fsolve(4*k^2*EllipticK(k)^2 = Eg, k = 0..1);
K := EllipticK(k);
V := 4*k^2*K^2*(2*JacobiSN[2*K*x, k]^2 - 1);
plot(V, x = 0..1);
curvature := 2*(1-k^2)*K^2/EllipticE(k)^2;
```

**APPENDIX C: DEPENDENCE OF CURVATURE $d^2E/dk^2|_{k=0}$ ON GAP WIDTH $\gamma_1$ FOR 1-GAP AND SINUSOIDAL POTENTIALS IN THE REGIMES OF SMALL AND LARGE $\gamma_1$**

The similarity between the $d^2E/dk^2|_{k=0}$ versus $\gamma_1$ curves shown in Fig. 7 for 1-gap (dashed curve) and sinusoidal (solid curve) potentials is not surprising. For small $\gamma_1$, by
consideration of Eqs. (24) and (29) for small \( m \) (Ref. 46, Sec. 17.3.11),

\[
\gamma_1 = \frac{\pi^2}{2} m^2 + \frac{\pi^2}{32} m^3 + \frac{17\pi^2}{64} m^4 + \cdots
\]  

(C1)

and

\[
\left. \frac{d^2 E}{dk^2} \right|_{k=0} = 2 - \frac{1}{4} m^2 - \frac{1}{4} m^3 - \frac{107}{512} m^4 + \cdots
\]  

(C2)

and hence

\[
\left. \frac{d^2 E}{dk^2} \right|_{k=0} = 2 - \frac{1}{4} \gamma_1^2 + \frac{104}{4096\pi^2} \gamma_1^4 + \cdots
\]  

(C3)

for a 1-gap potential. Similarly, from the expansions of \( a_1 \), \( b_1 \), and \( a \) for small \( q \) (Ref. 46, Secs. 20.2.25 25.3.15), it can be shown that

\[
\frac{d^2 E}{dk^2} \left|_{k=0} \right. = 2 - \frac{1}{4\pi^2} \gamma_1^2 + \frac{103}{4096\pi^2} \gamma_1^4 + \cdots
\]  

(C4)

for a sinusoidal potential, which matches the 1-gap series up to \( O(\gamma_1^2) \), and is very close up to \( O(\gamma_1^4) \).

For \( \gamma_1 \gg 1 \), it can be shown that

\[
\left. \frac{d^2 E}{dk^2} \right|_{k=0} \sim 8 \gamma_1 e^{\gamma_1} \]  

(C5)

for a 1-gap potential, and

\[
\left. \frac{d^2 E}{dk^2} \right|_{k=0} \sim \frac{2}{\pi^2} \gamma_1^{3/2} e^{-\gamma_1/\pi^2}
\]  

(C6)

for a sinusoidal potential. Hence, the 1-gap curvature tends to zero much more slowly than the sinusoidal potential curvature. Nevertheless, the absolute difference between curvatures will be very small for \( \gamma_1 \gg 1 \).
A turning point in $E(k)$ occurs if and only if $dE/dk=0$; i.e., $dk/dE$
is singular at that energy. From Eq. (25), this will happen at, and
only at, $E=\lambda_0$, and those band edges either side of gaps where
$\gamma>0$.


V. A. Marchenko and I. V. Ostrovskii, Mat. Sb. 97, 540 (1975)
[Mat. USSR. Sb. 26, 493 (1975)].

V. A. Marchenko, Sturm-Liouville Operators and Applications
3.4.

P. Kargaev and E. Korotyaev, unpublished.


Equation (9a) is derived from Eq. (2.15) in Ref. 40, after a change
of variables from $z$ to $E$ [Eq. (A3a)] and using $\mu_j$ instead of $\nu_j$
[Eq. (A5)]. Note that in Ref. 40, the $h_{-n}$ are deemed to be inde-
pendent from the $h_n$. For Hill’s equation, $h_{-n}=h_n$, and so Eq.
(9a) corresponds to $\partial_{-n}z+\partial_n z$ in Ref. 40 with $\nu_{-n}=\nu_n$ and
$z_{-n}=-z_n$.


Equation (22) follows from Ref. 50 after rescaling $x$ so that the
potential has period 1, shifting so that $\lambda_0=0$, and using parameter
$m$ instead of modulus $k$, as discussed in Appendix B.

M. Abramowitz and I. A. Stegun, Handbook of Mathematical

$m$ is the standard symbol used as parameter in the elliptic func-
tions and integrals. It should not be confused with the mass $m\tilde{m}$ of
Eq. (1) or the effective mass $m^*$ of Eq. (6).


E. T. Whittaker and G. N. Watson, A Course of Modern Analysis,


Wolfram Research, Inc., MATHEMATICA (Wolfram Research, Inc.,

Waterloo Maple, Inc., MAPLE (Waterloo Maple, Inc., Waterloo,
Ontario, 2001).

N. W. McLachlan, Theory and Application of Mathieu Functions


G. Yu, S. A. Studenikin, A. J. SpringThorpe, G. C. Aers, and D.
G. Austing, J. Appl. Phys. 97, 103703 (2005), and references
therein.


Appl. 16, 248 (1982)].


M. J. Ablowitz and A. S. Fokas, Complex Variables: Introduction
and Applications (Cambridge University Press, Cambridge,
1997), Cambridge Texts in Applied mathematics, Chap. 3.5.