Bandgap Extremization: Some Exact Results

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Abstract

We present here a variational method for maximizing the band gap in a one-dimensional system where the potential is subject to given constraints. Two specific examples are studied in detail. In the first, we show that if the potential is constrained to lie between two values, the largest bandgap is obtained by a mixture of the highest and lowest potential - an exact result valid in any dimension. The second example fixes the first and second moments of the potential and seeks to extremize the bandgap. An exact result is obtained. Finally, we indicate how our techniques may be applied to photonic bandgaps.

1 Introduction

Over the past decade, the design and study of photonic bandgap materials have attracted a lot of attention [1]. The design process often involves extremization of a bandgap with respect to variations in the dielectric constant profile in the material, subject to certain constraints. Materials so designed are expected to find use in optical communication. The theoretical work in this field lies in two broad areas: exact results that prove existence and provide bounds [2] and numerical algorithms that provide optimal designs [3]. In this paper we present a variational argument that provides criteria that the optimal design must satisfy, illustrated by two examples. (The calculations presented here are for quantum-mechanical bandgaps; however, the results are applicable also to the scalar Helmholtz equation - relevant for photonic band structure calculations - as indicated later.)

The first example leads us to a maximum contrast rule: if the potential is allowed to vary over a range of values, the optimal configuration is a combination of the largest and smallest values. The second example starts with a constraint on the second moment of the potential energy and leads to a sufficient (but not necessary) relationship between the wavefunction and the potential that - rather surprisingly - are satisfied by the solution we obtain. We verify the criteria and examine their consequences in one-dimension. Our exact results may be used as benchmarks in testing numerical algorithms and as tests for sharpness of proposed bounds.

We begin with the Schrödinger equation

\[- \nabla^2 \psi + v \psi = \epsilon \psi.\] (1)

Upon imposing appropriate boundary conditions on the wavefunction \(\psi\), this selects the energy eigenvalues \(\epsilon_n\) and eigenfunctions \(\psi_n\). We assume \(v\) to be real, and thus we can choose \(\psi_n\) to be real.

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The index $n = 0, 1, 2, \ldots$ orders the energy levels, so $\epsilon_{n+1} \geq \epsilon_n$. In one dimension with $\psi$ real, this index $n$ can be taken to be the number of nodes in the wavefunction, or equivalently the winding number in the $\psi - \psi'$ phase plane. In this paper - especially when we perform explicit calculations - we shall henceforth assume one dimension unless otherwise stated.

We now wish to consider the following sort of question: What potential $v$ - subject to constraints - gives a maximum $\epsilon_n$ for a particular state $n$? More elaborate questions will be considered shortly.

What type of constraints on the potential are we interested in? Since adding a constant $v(\vec{r}) \to v(\vec{r}) + v_0$ gives the trivial extension $\epsilon_n \to \epsilon_n + v_0$, the first constraint on $v$ should probably be to fix the average of $v$, so

$$\langle v \rangle = \int d\tau v(\vec{r}) = v_1. \quad (2)$$

The next constraint should limit the overall deviations from the average, and two reasonable choices might be to fix:

1. the second moment, so
   $$\langle v^2 \rangle = \int d\tau v^2(\vec{r}) = v_2. \quad (3)$$

2. the maximum contrast, so
   $$v_{\text{max}} \geq v(\vec{r}) \geq v_{\text{min}}. \quad (4)$$

In general, we assume a set of $J$ constraints of the form

$$G_j[v] = \int d\tau g_j[v] = v_j, \quad j = 1, 2, \ldots, J. \quad (5)$$

(The maximum contrast constraint can be cast into this form by an appropriate limiting $g[v]$; however, as we shall see, there are more direct methods.)

Now suppose we have solved the Schrödinger equation (1). We now make a small perturbation of the form

$$v(\vec{r}) \to v(\vec{r}) + \delta v(\vec{r}). \quad (6)$$

We evaluate the effect of this perturbation on the energy eigenvalue, to first order:

$$\delta \epsilon_n \approx \langle \delta v \rangle_n. \quad (7)$$

If we seek $\epsilon_n$ to be an extremum then we require our original state to satisfy

$$0 = \langle \delta v \rangle_n = \int d\tau \delta v \psi_n^2 \quad (8)$$

for any allowed variation $\delta v$. As an example of constraints, let us fix the first and second moments of $v$; then we require

$$0 = \int d\tau \delta v \quad (9)$$

$$0 = \int d\tau v \delta v. \quad (10)$$

Thus, (8) can be satisfied in general if

$$\psi_n^2 = \alpha + \beta v, \quad (11)$$

or

$$v = a + b\psi_n^2. \quad (12)$$

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This allows us to close the equations by solving the non-linear Schrödinger equation

\[- \nabla^2 \psi_n + [a + b \psi_n^2] \psi_n = \epsilon_n \psi_n. \tag{13}\]

The solution of the Schrödinger problem with the maximum contrast constraint is even easier, since we see from (8) that to maximize \( \epsilon_n \) we must choose

\[ v = \begin{cases} v_{\text{max}}, & \text{where } \psi_n^2 > \phi^2 \\ v_{\text{min}}, & \text{where } \psi_n^2 < \phi^2. \end{cases} \tag{14}\]

The constant \( \phi \) is chosen by imposing the first moment constraint.

In general, then, \( \langle \delta v \rangle_n = 0 \) is satisfied by choosing

\[ \psi_n^2 = \sum_{j=1}^J \alpha_j \frac{dg_j[v]}{dv}. \tag{15}\]

This equation can be inverted for \( v \), giving \( v = h[\psi_n^2 | \alpha] \), where \( \alpha \) represents the set of \( J \) parameters \( \alpha_j \). We then solve appropriate non-linear equations:

\[- \nabla^2 \psi_n + h[\psi_n^2 | \alpha] \psi_n = \epsilon_n \psi_n. \tag{16}\]

In this paper, we wish to maximize not the energy eigenvalues of the Schrödinger equation itself, but rather the energy bandgap between two levels, subject to constraints on the potential similar to previously. However, the constraints on the average of \( v \) is not really necessary, since we consider only bandgaps. (Note that the indices on \( \psi \) no longer refer to their ordering. In fact, we usually require that \( \psi_2, \psi_1 \) refer to consecutive eigenstates \( \psi_{n+1}, \psi_n \), and so for periodic boundary conditions in one dimension, these wavefunctions - the \textit{band edges} - will have exactly the same number of nodes.)

Thus, requiring the bandgap to be an extremum with respect to constrained variations of \( v \), we now have the following three coupled equations:

\[- \nabla^2 \psi_2 + v \psi_2 = \epsilon_2 \psi_2 \tag{17} \]
\[- \nabla^2 \psi_1 + v \psi_1 = \epsilon_1 \psi_1 \tag{18} \]
\[ \psi_2^2 - \psi_1^2 = \sum_{j=1}^J \alpha_j \frac{dg_j[v]}{dv}. \tag{19} \]

Again, we can invert to find \( v \), and rewrite the problem as two coupled non-linear Schrödinger equations

\[- \nabla^2 \psi_2 + h[\psi_2^2 - \psi_1^2 | \alpha] \psi_2 = \epsilon_2 \psi_2 \tag{20} \]
\[- \nabla^2 \psi_1 + h[\psi_2^2 - \psi_1^2 | \alpha] \psi_1 = \epsilon_1 \psi_1. \tag{21} \]

These equations are no longer quite so simple. We now consider our previous examples, in one dimension.

2 Two examples

2.1 Maximum contrast constraint

Without loss of generality, we reformulate the maximum contrast constraint as \( v_0 \geq v(x) \geq 0 \). Then returning directly to (8), we find

\[ \delta(\epsilon_2 - \epsilon_1) = \int dx [\psi_2^2 - \psi_1^2] \delta v \leq 0 \tag{22} \]
with no constraint on the average of $v$. Clearly the solution is

$$v(x) = \begin{cases} 
  v_0, & \text{if } \psi_2^2(x) > \psi_1^2(x) \\
  0, & \text{if } \psi_2^2(x) < \psi_1^2(x).
\end{cases} \quad (23)$$

Furthermore, we fix $v(x)$ to be periodic with period $L$, and designate $\psi_1$ and $\psi_2$ as each having one node per period (of $v(x)$). In other words, the two selected wavefunctions are at the band edges with Bloch wave vector $k = \frac{\pi}{L}$. The sole adjustable parameter left in the potential is the width of the ‘barrier’ of height $v_0$, which we call $2A$ ($0 \leq A \leq L/2$). Thus, we have:

$$v(x) = \begin{cases} 
  0, & -A < x < A \\
  v_0, & A < x < L - A
\end{cases}$$

extended periodically. Symmetry dictates that $\psi_1$ has nodes at $x = mL$ and $\psi_2$, at $x = (n + \frac{1}{2})L$ (or vice versa) where $m, n$ are integers. Therefore,

$$\psi_1(x) = \begin{cases} 
  \cos(k_1x), & -A < x < A \\
  a_1 \sinh[k_1(x - \frac{L}{2})], & A < x < L - A
\end{cases}$$

and

$$\psi_2(x) = \begin{cases} 
  \sin(k_2x), & -A < x < A \\
  a_2 \cosh[k_2(x - \frac{L}{2})], & A < x < L - A
\end{cases}$$

both extended periodically. Here $k^2 + \kappa^2 = v_0$ and $a_i$ are constants that ensure matching at the boundaries and may be eliminated to give:

$$y_1 \tan y_1 = \sqrt{\frac{\eta^2}{\alpha^2} - y_1^2} \coth \left( \left( \alpha - 1 \right) \sqrt{\frac{\eta^2}{\alpha^2} - y_1^2} \right) \quad \text{(24)}$$

and

$$\frac{\tan y_2}{y_2} = -\frac{1}{\sqrt{\frac{\eta^2}{\alpha^2} - y_2^2}} \coth \left( \left( \alpha - 1 \right) \sqrt{\frac{\eta^2}{\alpha^2} - y_2^2} \right) \quad \text{(25)}$$

where $y_i \equiv k_i A$, $\alpha \equiv L/2A$ and $\eta \equiv \sqrt{v_0} L/2$. The variables to be solved for are $y_1, y_2$ and $\alpha$. A third equation is provided by (23) which implies that $\psi_1^2(x) = \psi_2^2(x)$ at $x = A$ (and $x = L - A$):

$$\cot^2 y_1 \left( 1 - \frac{\left( \alpha - 1 \right) y_1^2}{\alpha^2 - y_1^2} \right) - \cot y_1 \frac{y_1^2}{y_1^2} \left( 1 + \frac{\left( \alpha - 1 \right) \eta^2}{\alpha^2 - y_1^2} \right)$$

$$= \tan^2 y_2 \left( 1 - \frac{\left( \alpha - 1 \right) y_2^2}{\alpha^2 - y_2^2} \right) + \tan y_2 \frac{y_2^2}{y_2^2} \left( 1 + \frac{\left( \alpha - 1 \right) \eta^2}{\alpha^2 - y_2^2} \right) \quad \text{(26)}$$

The solutions to these equations are displayed in the figures. Fig. 1 is a simultaneous plot of $\rho_1(A)$, $\rho_2(A)$ and $(\epsilon_2 - \epsilon_1)L^2/4$ against $\alpha$ at $\eta = 5$. Consistent with expectation, the energy difference is an extremum (maximum, in this case) when $\rho_1(A) = \rho_2(A)$, at $\alpha = 3.136$; Fig. 2 is a simultaneous plot of $\psi_1$, $\psi_2$ and $v(x)$ for this set of parameter values. Fig. 3 shows $\eta^2 (= v_0 L^2/4)$ against $1/\alpha (= 2A/L)$. The breaks in the plot are a consequence of poor convergence of the numerical routine used as $\kappa \geq 2$ and then $\kappa_1$ switch from imaginary to real with increasing $\eta$. Fig. 4 shows $\epsilon_1 L^2/4$, $\epsilon_2 L^2/4$ and (for reference) $v_0 L^2/4$ against $v_0 L^2/4$. Finally, Fig. 5 shows the energy difference (times $L^2/4$) in this case as well as for the potential $v(x) = v_0 \cos^2 \frac{\pi x}{L}$ for the same Bloch states, for comparison. (The latter has analytical eigenfunctions in terms of Mathieu functions.) As might be expected, the difference is larger with our optimized choice of potential.
Figure 1: $\rho_1(A), \rho_2(A)$ and $(\epsilon_2 - \epsilon_1)L^2/4$ (dot-dash, dash and solid lines, respectively) against $\alpha$ at $\eta = 5$.

Figure 2: $\psi_1, \psi_2$ and $v$ ($v_0 = 1.5$) (dot-dash, dash and solid lines, respectively) against $2x/L$. 

Figure 3: $\eta^2 = v_0L^2/4$ against $1/\alpha = 2A/L$.

Figure 4: $\epsilon_1L^2/4, \epsilon_2L^2/4$ (lower and upper solid lines, respectively) and $v_0L^2/4$ against $v_0L^2/4$. 
Figure 5: Size of bandgap (times $L^2/4$) against $v_0L^2/4$ for the optimized periodic square-well (solid line) and a sinusoidal potential with the same period and contrast (dashed line).

### 2.2 Second moment constraint

The equations we are to solve are

\begin{align*}
-\psi''_2 + v\psi_2 &= \epsilon_2\psi_2 \\
-\psi''_1 + v\psi_1 &= \epsilon_1\psi_1 \\
\psi_2^2 - \psi_1^2 &= \alpha v.
\end{align*}

We proceed with a roundabout strategy to solve these coupled equations by first solving the pair of coupled equations:

\begin{align*}
-\psi'' + v\psi &= \epsilon\psi \\
\psi^2 &= \beta v.
\end{align*}

This is equivalent to the single equation

\begin{equation}
\psi'' - \psi^3/\beta + \epsilon\psi = 0,
\end{equation}

which is (33) is one dimension. Suppose we find two such solutions with the same $v$, yet independent. Then we also have a solution to (27), with $\alpha = \beta_2 - \beta_1$. Clearly this gives a solution, but is it possible? The answer, as we demonstrate explicitly below, is yes.

We anticipate a periodic potential (with period $L$) and further impose the condition that the two energy eigenstates we seek are at the band edges, with period $2L$ for both. (The eigenfunctions may, then, be chosen to be real.) The solutions to (32) have remarkable properties [5, 7], one of which is exploited here. The equation may be solved in terms of the (periodic) Jacobian elliptic functions $sn$ or $cn$. (The third possibility, $dn$, turns out not to be appropriate.) We may now specifically require that the period of the potential be $L$. We finally obtain:

\begin{align*}
\psi_2(x) &= \frac{k}{\sqrt{L(1 - E/K)}} \text{sn}\left(\frac{2Kx}{L}\right) \\
\psi_1(x) &= \frac{k}{\sqrt{L(1 - E/K)}} \text{cn}\left(\frac{2Kx}{L}\right) \\
\frac{(\epsilon_2 - \epsilon_1)L^2}{4} &= (kK)^2
\end{align*}
where $E$ and $K$ are the complete elliptic integrals of modulus $k$. Note that $v$ is linearly related to both $\psi_1^2$ and $\psi_2^2$. Defining $\sigma^2 \equiv \frac{1}{L} \int_0^L dx \left( v^2 - \langle v \rangle^2 \right)$, we have

$$\sigma L^2 = 8K^2 \sqrt{\frac{2(1+k^2)(1-E/K) - k^2 - 3(1-E/K)^2}{3}}.$$  

(34)

It is, perhaps, useful to think of the whole system as being parametrized by $k$. The suitably scaled energy difference and strength of the potential (as $\sigma$) may be easily obtained from equations (33) and (34), respectively. Fig.6 shows $(\epsilon_2 - \epsilon_1) L^2 / 4$ against $\sigma L^2 / 4$ for the optimized potential (solid line), a sinusoidal potential with the same period and second moment (dot-dashed line) and the periodic square-well optimized (to a different criterion) in the previous example (dashed line).

3 Conclusion

We have discussed strategies for bandgap extremization subject to two very different, but realistic, constraints on the potential energy function. Our conclusions, in both cases, are illustrated by one-dimensional examples. It is worthwhile pointing out that the variational argument in the first example applies explicitly in any dimension. The second relies on the serendipitous existence of two solutions to the equations (27) in one dimension. Whether this stroke of luck can be replicated in higher dimensions is, to our knowledge, an open question.

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References

[1] Numerous references are available at http://home.earthlink.net/~jpdowling/pbgbib.html.

[2] M. S. Ashbaugh et al., Pacific J. Math. 147, 1 (1991).
   A. Figotin and P. Kuchment, SIAM J. Appl. Math. 56, 68 (1996).
A unified framework that applies to both the Schrödinger and Helmholtz equations starts with the general Schrödinger equation with parameter $c$:

$$-\nabla^2 \psi + cv \psi = \epsilon \psi.$$ 

The energy eigenvalues $\epsilon_n(c)$ are a family of functions parametrized by $c$. With the identification $v \rightarrow \rho$, $\psi \rightarrow u$ and identical boundary conditions, we can solve the Helmholtz equation

$$\nabla^2 u + \omega^2 \rho u = 0$$

by evaluating the roots of the equations $\epsilon_n(-\omega_n^2) = 0$. The variational techniques outlined in the paper may be applied to these equations as well. A detailed account will be presented in a forthcoming paper.