Homogenization theory for periodic potentials in the Schrödinger equation – Supplementary Material

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Abstract

This is a companion document to our journal article of the same title. We provide detailed proofs for the results stated in the main article. These calculations would be of use in a classroom setting, where they could serve as detailed and challenging exercises. In a second section of this companion document, we also give details of the MATLAB script used to compute the eigenvalues of the Bloch spectral cell problem.

1 Details of the calculations described in the main paper

The first calculation herein relates to a comment in the main paper that the results of the homogenization theory depend on the correct choice of scaling for the non-dimensional parameters α and β (these measure the strength of the periodic and large-scale potentials respectively). Here, we demonstrate that choosing $\alpha = 1/\varepsilon$ and $\beta = 0$, together with a time derivative that incorporates only large-scale temporal variations does not lead to a band-gap structure, but rather results in a net downward shift of all the energy levels, relative to the free-electron. The calculation can also be viewed as a full solution to problem 15, Chapter 12 in Reference [1].

Theorem 1 *Consider the following non-dimensional Schrödinger equation,*

$$\lambda\psi_\varepsilon = -\frac{\partial^2\psi_\varepsilon}{\partial x^2} + \frac{1}{\varepsilon}V_0\left(\frac{x}{\varepsilon}\right)\psi_\varepsilon, \qquad x \in (0,1), \tag{1}$$

with periodic boundary conditions $\psi_\varepsilon(x = 0) = \psi_\varepsilon(x = 1)$. Let λ be an $O(1)$ eigenvalue, and let $V_0(\cdot)$ be a continuous 1-periodic function on $[0, 1]$. Then, standard homogenization theory leads to a homogenized Schrödinger equation whose energy levels are less than the 'free' case (i.e. $V_0 = 0$).

Proof: We follow standard practice in homogenization theory and treat x and $y := x/\varepsilon$ as independent large-scale and small-scale variations respectively, such that the spatial derivative becomes.

$$\frac{\partial}{\partial x} \to \frac{\partial}{\partial x} + \frac{1}{\varepsilon}\frac{\partial}{\partial y}. \tag{2}$$

We replace $\psi_\varepsilon(x)$ with $\psi(x,y)$, a function of two variables, and expand the latter in powers of ε:

$$\psi(x,y) = \sum_{p=0}^{\infty} \varepsilon^p \psi_p(x,y). \tag{3}$$

Substitution of this expansion into Equation (1) yields

$$-\left(\frac{\partial^2}{\partial x^2} + \frac{2}{\varepsilon}\frac{\partial^2}{\partial x \partial y} + \frac{1}{\varepsilon^2}\frac{\partial^2}{\partial y^2}\right)\sum_{p=0}^{\infty} \varepsilon^p \psi_p(x,y) + \frac{1}{\varepsilon} V_0(y) \sum_{p=0}^{\infty} \varepsilon^p \psi_p(x,y) = \lambda \sum_{p=0}^{\infty} \varepsilon^p \psi_p(x,y). \tag{4}$$

We equate the terms arising from each order in the power-series expansion. At $O(\varepsilon^{-2})$, we have

$$\frac{\partial^2 \psi_0}{\partial y^2} = 0, \tag{5}$$

hence $\psi_0 = \psi_0(x)$ alone. At $O(\varepsilon^{-1})$, the result reads

$$-2\frac{\partial^2 \psi_0}{\partial x \partial y} - \frac{\partial^2 \psi_1}{\partial y^2} + V_0(y)\psi_0 = 0. \tag{6}$$

Using $\psi_0 = \psi_0(x)$, this becomes

$$\frac{\partial^2 \psi_1}{\partial y^2} = V_0(y)\psi_0(x). \tag{7}$$

We assume without loss of generality that the potential has zero mean. This amounts to choosing a particular reference level for the potential function. Then, Equation (7) has solution

$$\psi_1(x,y) = \psi_0(x)\frac{\partial^{-2} V_0}{\partial y^{-2}},$$

where

$$\frac{\partial^{-2} V_0}{\partial y^{-2}} := -\frac{1}{4\pi^2}\sum_{n=1}^{\infty} \frac{1}{n^2}\left[a_n \cos(2\pi n y) + b_n \sin(2\pi n y)\right],$$

and where a_n and b_n are the Fourier coefficients of the periodic potential $V_0(y)$ (the coefficient a_0 is zero because V_0 has mean zero). Finally, at $O(1)$, we have

$$-\frac{\partial^2 \psi_0}{\partial x^2} - 2\frac{\partial^2 \psi_1}{\partial x \partial y} - \frac{\partial^2 \psi_2}{\partial y^2} + V_0(y)\psi_1 = \lambda \psi_0. \tag{8}$$

We average Equation (8) over the small-scale variations to obtain

$$-\frac{\partial^2 \psi_0}{\partial x^2} + \langle V_0(y)\psi_1(x,y)\rangle = \lambda \psi_0, \tag{9}$$

where $\langle\cdot\rangle = \int_0^1 (\cdot)\,\mathrm{d}y$ denotes averaging. It remains to compute the term $\langle V_0(y)\psi_1(x,y)\rangle$:

$$\begin{aligned}
\langle V_0(y)\psi_1(x,y)\rangle &= \int_0^1 V_0(y)\psi_1(x,y)\mathrm{d}y, \\
&= \psi_0(x)\int_0^1 V_0(y)\frac{\partial^{-2}V_0}{\partial y^{-2}}\mathrm{d}y, \\
&= -\psi_0(x)\int_0^1 \left(\frac{\partial^{-1}V_0}{\partial y^{-1}}\right)^2 \mathrm{d}y, \\
&= -\psi_0(x)\int_0^1 \left\{\sum_{n=1}^{\infty}\frac{1}{2\pi n}\left[a_n\sin(2\pi n y) - b_n\cos(2\pi n y)\right]\right\}^2 \mathrm{d}y, \\
&= -\psi_0(x)\sum_{n=1}^{\infty}\frac{1}{8\pi^2 n^2}\left(a_n^2 + b_n^2\right), \\
&:= -D\psi_0(x),
\end{aligned}$$

where D is a positive constant. The homogenized equation (9) therefore reads

$$-\frac{\partial^2\psi_0}{\partial x^2} - D\psi_0 = \lambda\psi_0. \tag{10}$$

We solve this in a standard fashion, with periodic boundary conditions $\psi = 0$ at $x = 0, 1$. The result is $\psi_0(x) = (2\pi)^{-1/2}\mathrm{e}^{2\pi\mathrm{i}nx}$, with $n \in \mathbb{Z}$. Thus,

$$\lambda_n = 4\pi^2 n^2 - D,$$

and $\lambda_n \leq 4\pi^2 n^2$, such that the energy levels undergo a downward shift relative to the solution for the free-particle ($V_0 = 0$) calculation. ∎

Theorem 2 *The Bloch spectral-cell problem defined in the main paper, viz.*

$$\lambda f(y;k) = -\left(\frac{\partial}{\partial y} + \mathrm{i}k\right)^2 f(y;k) + V_0(y)f(y;k), \qquad f(0;k) = f(1;k), \tag{11}$$

is self-adjoint.

Proof: Since $V_0(y)$ in Equation (11) is a a potential energy, it is a real-valued function. Thus, it suffices to show that the operator $(d/dy + \mathrm{i}k)^2$ is self-adjoint. Thus, let f and g be complex-valued functions of the single real-variable y, periodic on the interval $[0, 1]$. The inner product of f and g is defined in the usual way:

$$\langle f, g\rangle := \int_0^1 f^* g\,\mathrm{d}y.$$

We compute $\langle f, (d/dy + \mathrm{i}k)^2 g\rangle$, and use integration by parts (I.B.P.) repeatedly. Moreover, we use the fact that the boundary conditions are periodic, such that

boundary terms in the integration by parts vanish. We have,

$$\begin{aligned}
\langle f, (d/dy + \mathrm{i}k)^2 g\rangle &= \int_0^1 f^* \left(\frac{d}{dy} + \mathrm{i}k\right)^2 g \,\mathrm{d}y, \\
&= \int_0^1 f^* \left(\frac{d^2 g}{dy^2} + 2\mathrm{i}k\frac{dg}{dy} - k^2 g\right) \mathrm{d}y, \\
&\overset{\text{I.B.P.}}{=} \int_0^1 \left(\frac{d^2 f^*}{dy^2} - 2\mathrm{i}k\frac{df^*}{dy} g - k^2 f^* g\right) \mathrm{d}y, \\
&= \int_0^1 \left[\frac{d^2 f^*}{dy^2} + \frac{d}{dy}(2\mathrm{i}kf)^* - k^2 f^*\right] g \,\mathrm{d}y, \\
&= \int_0^1 \left[\left(\frac{d}{dy} + \mathrm{i}k\right)^2 f\right]^* g \,\mathrm{d}y, \\
&= \langle (d/dy + \mathrm{i}k)^2 f, g\rangle. \quad \blacksquare
\end{aligned}$$

In the main paper, it was shown that the solution to the $O(\varepsilon^{-1})$ and $O(1)$ problems could be computed in terms of the Bloch functions for the particular case where $k = k_n$, where $(d\lambda/dk)_{k_n} = 0$. In particular, it was found that

$$u_1 = -\mathrm{i}\frac{\partial\phi}{\partial x}\frac{\partial f}{\partial k}\bigg|_{k_n}, \qquad u_2 = -\tfrac{1}{2}\frac{\partial^2\phi}{\partial x^2}\frac{\partial^2 f_n}{\partial k^2}\bigg|_{k_n}, \qquad k = k_n,$$

provided ϕ satisfies the following consistency condition:

$$\mathrm{i}\frac{\partial\phi}{\partial t} = -\tfrac{1}{2}\left(\frac{d^2\lambda_n}{dk^2}\right)_{k_n}\frac{\partial^2\phi}{\partial x^2} + V_{1,\text{eff}}(x)\phi(x), \tag{12a}$$

where

$$V_{1,\text{eff}}(x) = \int_0^1 \mathrm{d}y\, |f_n(y;k_n)|^2 V_1(x,y). \tag{12b}$$

We now prove the following theorem:

Theorem 3 *Let the spectral cell problem*

$$\lambda_n f_n(y;k) = -\left(\frac{\partial}{\partial y} + \mathrm{i}k\right)^2 f_n(y;k) + V_0(y) f_n(y;k), \qquad f_n(0;k) = f_n(1;k), \tag{13}$$

be non-degenerate. Introduce

$$\widetilde{\phi}(x,t) = \phi\left(x - \frac{1}{\varepsilon}\frac{d\lambda}{dt}t, t\right),$$

where $\phi(\cdot,\cdot)$ solves Equations (12)*. Then*

$$u_0 = \mathrm{e}^{-\mathrm{i}\lambda_n T} f_n(y;k)\widetilde{\phi}(x,t), \qquad u_1 = -\left(\mathrm{i}\frac{\partial\widetilde{\phi}}{\partial x}\frac{\partial f_n}{\partial k}\right)\mathrm{e}^{-\mathrm{i}\lambda_n T}, \qquad u_2 = -\left(\tfrac{1}{2}\frac{\partial^2\widetilde{\phi}}{\partial x^2}\frac{\partial^2 f_n}{\partial k^2}\right)\mathrm{e}^{-\mathrm{i}\lambda_n T},$$

solves the problem

$$\left(\frac{1}{\varepsilon^2}\mathcal{L}_0+\frac{1}{\varepsilon}\mathcal{L}_1+\mathcal{L}_2\right)\left(u_0+\varepsilon u_1+\varepsilon^2 u_2\right)=O(\varepsilon), \tag{14a}$$

where

$$\mathcal{L}_0 = \mathrm{i}\frac{\partial}{\partial T}-\left[-\left(\partial_y+\mathrm{i}k\right)^2+V_0(y)\right], \tag{14b}$$
$$\mathcal{L}_1 = -2\left(-\mathrm{i}k\partial_x-\partial_x\partial_y\right), \tag{14c}$$
$$\mathcal{L}_2 = \mathrm{i}\frac{\partial}{\partial t}-\left[-\partial_x^2+V_1(x,y)\right]. \tag{14d}$$

Proof: We expand the left-hand side of the problem (14a) explicitly:

$$\left(\frac{1}{\varepsilon^2}\mathcal{L}_0u_0\right)+\frac{1}{\varepsilon}\left(\mathcal{L}_1u_0+\mathcal{L}_0u_1\right)+\left(\mathcal{L}_2u_0+\mathcal{L}_1u_1+\mathcal{L}_0u_2\right)+\varepsilon\left(\mathcal{L}_2u_1+\mathcal{L}_1u_2\right)+\varepsilon^2\left(\mathcal{L}_2u_2\right).$$

The $O(\varepsilon^{-2})$ contribution to Equation (14a) reads

$$\mathrm{i}\frac{\partial u_0}{\partial T}=-\left(\frac{\partial}{\partial y}+\mathrm{i}k\right)^2u_0+V_0(y)u_0.$$

Clearly, this equation is solved by the ansatz $u_0=\mathrm{e}^{-\mathrm{i}\lambda_nT}f_n(y;k)\widetilde{\phi}(x,t)$ proposed in the statement of the theorem. We therefore consider the contributions to Equation (14a) at $O(\varepsilon^{-1})$. Care must be taken here, as this problem contains not only the terms $\varepsilon^{-1}\left(\mathcal{L}_1u_0+\mathcal{L}_0u_1\right)$, but also a contribution from the term $\mathcal{L}_2u_0$, since

$$\begin{aligned}
\varepsilon\mathcal{L}_2u_0 &= \mathrm{i}\varepsilon\frac{\partial}{\partial t}\left[\mathrm{e}^{-\mathrm{i}\lambda_nT}f_n(y;k)\widetilde{\phi}\left(x-\frac{1}{\varepsilon}\frac{d\lambda_n}{dk}t,t\right)\right]\\
&\qquad -\varepsilon\left[-\partial_x^2+V_1(x,y)\right]\mathrm{e}^{-\mathrm{i}\lambda_nT}f_n(y;k)\widetilde{\phi}\left(x-\frac{1}{\varepsilon}\frac{d\lambda_n}{dk}t,t\right),\\
&= \mathrm{i}\varepsilon\mathrm{e}^{-\mathrm{i}\lambda_nT}f_n(y;k)\left(-\frac{1}{\varepsilon}\frac{d\lambda_n}{dk}\frac{\partial\widetilde{\phi}}{\partial x}+\frac{\partial\widetilde{\phi}}{\partial t}\right)+O(\varepsilon),\\
&= -\mathrm{i}\mathrm{e}^{-\mathrm{i}\lambda_nT}f_n(y;k)\frac{d\lambda_n}{dk}\frac{\partial\widetilde{\phi}}{\partial x}+O(\varepsilon),\\
\mathcal{L}_2u_0 &= -\frac{1}{\varepsilon}\mathrm{i}\mathrm{e}^{-\mathrm{i}\lambda_nT}f_n(y;k)\frac{d\lambda_n}{dk}\frac{\partial\widetilde{\phi}}{\partial x}+O(\varepsilon^0),
\end{aligned} \tag{15}$$

Next, we make the replacement $\partial/\partial T\to-\mathrm{i}\lambda_n$. This is legitimate, as the eigenstates are one-dimensional; hence, time derivatives in a particular eigenstate correspond unambiguously to a single eigenfunction. Using these results, and the definitions of $\mathcal{L}_0$ and $\mathcal{L}_1$, the problem (14a) at $O(\varepsilon^{-1})$ reads

$$\lambda_nu_1-\underline{f_n\frac{\partial\widetilde{\phi}}{\partial x}\frac{d\lambda_n}{dk}}=-\left(\frac{\partial}{\partial y}+\mathrm{i}k\right)^2u_1+V_0(y)u_1-2\mathrm{i}kf_n\frac{\partial\widetilde{\phi}}{\partial x}-2\frac{\partial f_n}{\partial y}\frac{\partial\widetilde{\phi}}{\partial x}, \tag{16}$$

where the underlined term comes from the chain-rule calculation (15). We propose the trial solution $u_1 = g(y;k)(\partial\widetilde{\phi}/\partial x)$. Substitution of this ansatz into (16) yields

$$\lambda_n g - \mathrm{i} f_n \frac{d\lambda_n}{dk} = -\left(\frac{\partial}{\partial y} + \mathrm{i}k\right)^2 g + V_0(y) g - 2\mathrm{i}k f_n - 2\frac{\partial f_n}{\partial y}.$$

On the other hand, consider the derivative of the Bloch spectral cell problem (13) with respect to k:

$$\frac{d\lambda_n}{dk} f_n + \lambda_n \frac{\partial f_n}{\partial k} = -\left(\frac{\partial}{\partial y} + \mathrm{i}k\right)^2 \frac{\partial f_n}{\partial k} + V_0(y)\frac{\partial f_n}{\partial k} - 2\mathrm{i}\left(\frac{\partial}{\partial y} + \mathrm{i}k\right) f_n$$

Comparison of these two equations yields $g(x,t) = -\mathrm{i}(\partial f_n/\partial k)$ and $u_1 = -\mathrm{i}(\partial f_n/\partial k)(\partial\widetilde{\phi}/\partial x)$. The temporal dependence on the rapid timescale T is restored by multiplication of this solution by the appropriate phase:

$$u_1 = -\mathrm{i}\left(\frac{\partial f_n}{\partial k}\frac{\partial\widetilde{\phi}}{\partial x}\right)\mathrm{e}^{-\mathrm{i}\lambda_n T}.$$

Finally, consider the $O(1)$ contribution to Equation (14a). Using the fact that $u_1 = -\mathrm{i}(\partial f_n/\partial k)(\partial\widetilde{\phi}/\partial x)$, and the chain rule, it follows that

$$\frac{\partial u_1}{\partial t_1} = -\mathrm{i}\frac{\partial f_n}{\partial k}\left(-\frac{1}{\varepsilon}\frac{\partial^2\widetilde{\phi}}{\partial x^2}\frac{d\lambda_n}{dk} + \frac{\partial^2\widetilde{\phi}}{\partial x \partial t_1}\right). \tag{17}$$

Hence, the term $\mathcal{L}_2 u_1$ contributes to the $O(1)$ problem, which now reads

$$\lambda u_2 - \underline{\frac{\partial f_n}{\partial k}\frac{d\lambda_n}{dk}\frac{\partial^2\widetilde{\phi}}{\partial x^2}} + \mathrm{i}f_n\frac{\partial\widetilde{\phi}}{\partial t_1} = -f_n\frac{\partial^2\widetilde{\phi}}{\partial x^2} + V_1(x,y)f_n\widetilde{\phi} - \left(\frac{\partial}{\partial y} + \mathrm{i}k\right)^2 u_2 + V_0(y)u_2 - 2\mathrm{i}k\frac{\partial u_1}{\partial x} - 2\frac{\partial^2 u_1}{\partial x \partial y}, \tag{18}$$

where the underlined term arises because of the application (17) of the chain rule. We substitute the $O(\varepsilon^{-1})$ solutions into Equation (18). This yields

$$\lambda_n u_2 - \frac{\partial f_n}{\partial k}\frac{d\lambda_n}{dk}\frac{\partial^2\widetilde{\phi}}{\partial x^2} + \mathrm{i}f_n\frac{\partial\widetilde{\phi}}{\partial t_1} = -f_n\frac{\partial^2\widetilde{\phi}}{\partial x^2} + V_1(x,y)f_n\widetilde{\phi} - \left(\frac{\partial}{\partial y} + \mathrm{i}k\right)^2 u_2 + V_0(y)u_2 - 2k\frac{\partial f_n}{\partial k}\frac{\partial^2\widetilde{\phi}}{\partial x^2} + 2\mathrm{i}\frac{\partial^2 f_n}{\partial y \partial k}\frac{\partial\widetilde{\phi}}{\partial x^2}.$$

We make the trial solution $u_2 = h(y;k)(\partial^2\widetilde{\phi}/\partial x^2)$, such that

$$\lambda_n h\frac{\partial^2\widetilde{\phi}}{\partial x^2} - \frac{\partial f_n}{\partial k}\frac{d\lambda_n}{dk}\frac{\partial^2\widetilde{\phi}}{\partial x^2} + \mathrm{i}f_n\frac{\partial\widetilde{\phi}}{\partial t_1} = -f_n\frac{\partial^2\widetilde{\phi}}{\partial x^2} + V_1(x,y)f_n\widetilde{\phi} - \frac{\partial^2\widetilde{\phi}}{\partial x^2}\left(\frac{\partial}{\partial y} + \mathrm{i}k\right)^2 h - 2k\frac{\partial f_n}{\partial k}\frac{\partial^2\widetilde{\phi}}{\partial x^2} + 2\mathrm{i}\frac{\partial^2 f_n}{\partial y \partial k}\frac{\partial\widetilde{\phi}}{\partial x^2}. \tag{19}$$

On the other hand, consider also the second derivative of the spectral cell equation (13) with respect to k:

$$\lambda\frac{\partial^2 f_n}{\partial k^2}+2\frac{\partial f_n}{\partial k}\frac{d\lambda_n}{dk}+f_n\frac{\partial^2\lambda}{\partial k^2}=V_0(y)\frac{\partial^2 f_n}{\partial k^2}-\left(\frac{\partial}{\partial y}+\mathrm{i}k\right)^2\frac{\partial^2 f_n}{\partial k^2}-4\mathrm{i}\left(\frac{\partial}{\partial y}+\mathrm{i}k\right)\frac{\partial f_n}{\partial k}+2f_n. \tag{20}$$

Comparing Eqs. (19) and (20) yields

$$u_2=-\tfrac{1}{2}\frac{\partial^2 f_n}{\partial k^2}\frac{\partial\widetilde{\phi}}{\partial x^2},$$

provided the consistency condition

$$\mathrm{i}\frac{\partial\widetilde{\phi}}{\partial t_1}f_n(y;k)=-\tfrac{1}{2}\frac{d^2\lambda_n}{dk^2}\frac{\partial^2\widetilde{\phi}}{\partial x^2}f_n(y;k)+V_1(x,y)\widetilde{\phi}f_n(y;k) \tag{21}$$

is satisfied. We multiply Equation (21) by f_n^* and integrating the result over all $y\in[0,1]$. Since the f_n's are orthonormal eigenfunctions on this interval, this integration yields

$$\mathrm{i}\frac{\partial\widetilde{\phi}}{\partial t_1}=-\frac{1}{2m_{\mathrm{eff}}}\frac{\partial^2\widetilde{\phi}}{\partial x^2}+V_{1,\mathrm{eff}}(x)\widetilde{\phi},$$

where

$$m_{\mathrm{eff}}=\left(\tfrac{1}{2}\frac{d^2\lambda_n}{dk^2}\right)^{-1},$$

and

$$V_{1,\mathrm{eff}}(x)=\int_0^1|f_n(y;k)|^2V_1(x,y)\mathrm{d}y.$$

Again, the temporal dependence on the rapid timescale T is restored by multiplication of this solution by the appropriate phase:

$$u_2=-\left(\tfrac{1}{2}\frac{\partial^2 f_n}{\partial k^2}\frac{\partial\widetilde{\phi}}{\partial x^2},\right)\mathrm{e}^{-\mathrm{i}\lambda_n T}. \qquad \blacksquare$$

The final theorem in this companion document concerns an application of Hölder's inequality to the effective-mass calculation in the Sec. V of the main paper, wherein it is shown that

$$m_{\mathrm{eff}}(n=0,k=0)\geq m,$$

where m is the ordinary inertial mass.

Theorem 4 *Let $f:[0,1]\to\mathbb{R}$ be a continuous, strictly positive function on $[0,1]$: $f(x)>0$, for all $x\in[0,1]$. Then $1/f$ is integrable and, moreover,*

$$\left(\int_0^1(1/f)\,\mathrm{d}x\right)^{-1}\leq\int_0^1 f\,\mathrm{d}x.$$

Proof: Since $f(x)$ is continuous on $[0,1]$ it is bounded and continuous on the same interval, and is therefore integrable. Moreover, since f is strictly positive on $[0,1]$, the function $1/f$ is bounded and continuous on the same interval, and is therefore integrable. Consider now Hölder's inequality for arbitrary integrable functions $a(x)$ and $b(x)$ on $[0,1]$:

$$\int_0^1 |ab|\,\mathrm{d}x \leq \|a\|_2 \|b\|_2,$$

where $\|\cdot\|_2 = (\int_0^1 (\cdot)^2\,\mathrm{d}x)^{1/2}$ is the usual L^2 norm. Since f is strictly positive, we set $a = f^{1/2}$ and $b = 1/f^{1/2}$ (both integrable functions) to obtain

$$1 \leq \|f^{1/2}\|_2 \|f^{-1/2}\|_2.$$

In other words,

$$1 \leq \left[\int_0^1 f\,\mathrm{d}x\right]^{1/2} \left[\int_0^1 (1/f)\mathrm{d}x\right]^{1/2}.$$

Squaring both sides and re-arranging the inequality yields

$$\left(\int_0^1 (1/f)\,\mathrm{d}x\right)^{-1} \leq \int_0^1 f\,\mathrm{d}x. \quad \blacksquare$$

2 Details of the numerical method described in the main paper

In this section we include the MATLAB '.m' file used to generate the first few eigenvalues $\lambda_0, \cdots, \lambda_{N-1}$ of the Bloch spectral cell problem (Equation (11) herein), for an arbitrary potential $V_0(y)$. The input parameters are k, the wavenumber, and N, the number of collocation points in the numerical method. The number N can be varied until the numerical method converges. The first output (labelled 'lambdas' in the code) is an array containing an approximation to the first N eigenvalues in the spectral cell problem, in increasing order. Typically, the lowest-energy eigenvalue is the most accurately-computed value, while the accuracy decreases as one accesses higher parts of the spectrum. However, a given large-energy eigenvalue can be computed to any level of accuracy by increasing N. The other two outputs are the matrices L and M described in the main paper.

```
function [lambdas,L_mx,M_mx] = make_all_matrices(k,N)

% This matlab function calculates the first N eigenvalues
% for a given input wavenumber k.

im=sqrt(-1);

% Create an array of spatial points, with resolution determined by N

jj = 1:(2*N+1);
yy = (0.5/(N+2))*jj;
```

```
% Define the periodic potential
uu = 5*sin(2*pi*yy);

L_mx = zeros(2*N+1);
M_mx = zeros(2*N+1);

for j = 1:(2*N+1)
    for n = -N:N
        m = n + N + 1;
        M_mx(j,m) = exp(2*pi*im*n*yy(j));
        L_mx(j,m) = ((2*pi*n+k)^2)*exp(2*pi*im*n*yy(j)) ...
           + uu(j)*exp(2*pi*im*n*yy(j));
    end
end

lambdas = eig(L_mx,M_mx);

% Check that the imaginary part of the eigenvalues is zero
% to machine precision, then make the reality of the eigenvalues
% explicit in the next line:

lambdas=real(lambdas);
lambdas=sort(lambdas);
```

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References

[1] G. Pavliotis and A. M. Stuart. *Multiscale Methods*. Springer, Berlin, 2008.