OPTI 571L Lab 14: Quantum motion in periodic potentials: From band structure to tight binding

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Wave propagation in periodic structures is ubiquitous in optical physics, a prime example being quantized motion of an electron in the periodic potential due to the ions in a metal, semiconductor, or insulator. But other examples abound involving matter waves including electron motion in quantum wells, the quantized motion of atoms in the periodic potential due to applied laser beams, and lattices of Bose-Einstein condensates each of which are tightly bound to an individual potential well. Examples in optics include electromagnetic waves in media with periodically modulated refractive index such as Bragg gratings, light propagation in quantum well structures, and light propagation in arrays of evanescently coupled single-mode waveguides.

The goal of this lab is to have you explore the concepts underlying these phenomena using the example of a quantum particle's motion in a periodic potential. In particular, you shall numerically solve the so-called Krönig-Penney model in one dimension using a matrix method [1], the potential for this exactly soluble model being a periodic array of rect-functions. The first example will involve the band structure and energy gaps that are foundational to all problems dealing wave propagation in periodic structures. Next you will examine the tight-binding limit in which the particles get concentrated or pinned around the various potential wells or lattice sites.

Keywords: Krönig-Penney model, numerical solution, band structure, Bloch waves, tight binding, quantum tunnelling.

I. KRÖNIG-PENNEY MODEL

Read pp. 426-428 of Ref. [1] to obtain a broad overview of the Krönig-Penny (KP) model. The Hamiltonian for the KP model of a quantum particle moving in one dimension is [1]

$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + V(x), \tag{1}$$

with μ the effective mass. The potential $V(x)$ is expressed as a sum of potential barriers in the form of rect-functions of full-width b with centers at equally spaced positions x_r separated by a distance $a > b$

$$V(x) = \sum_r V_0 \; rect\left(\frac{x - x_r}{b}\right), \quad (x_{r+1} - x_r) = a. \tag{2}$$

With $V_0 > 0$ the potential is therefore zero between barriers, and has value V_0 inside each potential barrier, the potential having the form of a periodic lattice. The time-independent Schrödinger equation is $\hat{H}\psi(x) = E\psi(x)$. The KP model is exactly soluble but here you shall solve it numerically.

A. Matrix method

The matrix method is based on the idea that the main properties of the periodic structure, in particular the energies, can be obtained by considering a finite number $n_b > 1$ of potential barriers of width b and centers at $x_r = (-a/2 + ra)$ with $r = 1, 2, \ldots n_b$: This is reasonable since physical systems are not infinite in extent, such as crystals with a finite number of unit cells, and photonic Bragg filters composed of a finite number of periods. The approach is then to solve the Schrödinger equation on the finite domain $x = [0, L]$ with $L = n_b a$.

The first step is to numerically solve the time-independent Schrödinger equation $\hat{H}\psi(x) = E\psi(x)$ with the box boundary conditions $\psi(0) = \psi(L) = 0$. One way to do this is to expand the wavefunction $\psi(x)$ into a set of basis modes $\{\varphi_p(x)\}$ that obey the boundary conditions. A particular choice is the set of box modes obtained with the periodic potential set to zero ($V_0 = 0$)

$$\varphi_m(x) = \sqrt{\frac{2}{L}} \sin\left(k_m x\right), \quad m = 1, 2, \ldots \tag{3}$$

where $k_m = \frac{m\pi}{L}$ is the wavevector for the mth basis mode. Then approximating the wavefunction for the full problem using N basis modes

$$\psi(x) \approx \sum_{m=1}^{N} c_m \varphi_m(x), \tag{4}$$

leads to the matrix form of the time-independent Schrödinger equation

$$\begin{pmatrix} H_{11} & H_{12} & \ldots & H_{1N} \\ H_{21} & H_{22} & \ldots & H_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ H_{N1} & H_{N2} & \ldots & H_{NN} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}, \tag{5}$$

where the matrix elements of the Hamiltonian are

$$H_{nm} = \delta_{nm} E_n^{(0)} + \int_0^L dx\ \varphi_n^*(x) V(x) \varphi_m(x)$$
$$= \delta_{nm} \left(\frac{\hbar^2 \pi^2 n^2}{2\mu L^2} \right) + \frac{2}{L} \int_0^L dx\ \sin\left(\frac{n\pi x}{L}\right) V(x) \sin\left(\frac{m\pi x}{L}\right). \quad (6)$$

Here the zeroth-order energies $E_n^{(0)}$ are the energy eigenvalues for the box in the absence of the periodic potential, that is, with $V_0 = 0$.

In what follows units are used such that $a = 1$ and $\hbar^2/2\mu = 1$, so that $L = n_b$, $x = [0, n_b]$, $x_r = (-1/2 + r)$, and all energies are in units of $\hbar^2/2\mu a^2 = 1$. Throughout this Lab set $n_b = 10, b = 1/6$, and $V_0 = 100$.

(a) Make sure you understand the derivation of the matrix Schrödinger Eq. (5) based on the material from the quantum class you took.

(b) To make sure you understand the geometry write a MATLAB code to plot $V(x)$ versus $x = [0, 10]$ using $n_x = 10000$ points. You should see 10 equally spaced potential barriers of height 100 each of width 1/6.

(c) One way to evaluate the Hamiltonian matrix elements H_{nm} is by direct numerical integration of Eq. (6). Write a MATLAB code to generate the matrix elements H_{nm} for $N = 100$ and the parameters in part (b), you have the code $V(x)$ from part (b). As a check some values are $H_{11} = 16.77, H_{33} = 17.55, H_{55} = 19.13$.

(d) This part is optional: An alternative way to obtain the Hamiltonian matrix elements H_{nm} is to use the analytic solution given in Eqs. (14-17) of Ref. [1]. You may choose this method if you wish, or you can use it as a test for part (c).

B. Band structure

In this section you shall examine the energy eigenvalues E_n of the matrix Schrödinger Eq. (5) that give rise to the band structure. Here the eignvalues should be organized such that $E_1 < E_2 < E_3$..., so that $n = 1$ is the ground state. For each eigensolution there is an associated wavevector $k_n = \frac{n\pi}{L}$, or in the scaled units $k_n = \frac{n\pi}{n_b}$. The scaled free-particle energies with the potential absent are $E_n^{(0)} = \pi^2 n^2 / n_b^2$.

(a) Write a MATLAB code that calculates the Hamiltonian matrix elements H_{nm}, and solve for the eigenvalues and eigenvectors using the MATLAB function `eigs` (see Sec. 1 of Lab 1). On the same figure plot the quantities (E_n/π^2) and $(E_n^{(0)}/\pi^2)$ versus $(k_n/\pi) = [1 : 1 : 29]/10$: Use a dashed curve for the free-particle case and circle symbols for the energy eigenvalues.

Your figure from part (a) should coincide with Fig. 2 of Ref. [1], and this corresponds to the band structure. You should see three energy bands that we label using the *band index* $j = 1, 2, \ldots$. For this example the first band ($j = 1$) has values $(k_n/\pi) = [1 : 1 : 9]/10$, this is within the first Brillouin zone, the second band ($j = 2$) has $(k_n/\pi) = [10 : 1 : 20]/10$, and the third band ($j = 3$) has $(k_n/\pi) = [21 : 1 : 29]/10$. You should see that an energy gap opens up around the edge of each Brillouin zone, where k/π is an integer, as you will have learned in your solid state physics classes. This is the *extended zone scheme*.

(b) There is also the reduced zone scheme in which the band structure is folded within the first Brillouin zone $(k/\pi) = [0, 1]$. In particular, for the first band ($j = 1$) $(k_n/\pi) = [1 : 1 : 9]/10$, for the second band ($j = 2$) $(k_n/\pi) = [10 : -1 : 0]/10$, and for the third band ($j = 3$) $(k_n/\pi) = [1 : 1 : 9]/10$. Using this information plot the band structure in the reduced zone scheme, using circle symbols to mark the data points. You should see a band structure of the type that is more familiar from solid state texts.

In the reduced zone scheme the band index j is needed in conjunction with the wavevector in the first Brillouin zone to specify a particular solution. In particular, in the vicinity of the Γ-point at $k = 0$ one can see an energy gap between the $j = 2$ and $j = 3$ bands that is akin to the band gap that appears in a semiconductor. Completing this exercise should clarify some of the notions underlying band structure as used in solid state.

C. Bloch standing waves

Next you shall evaluate the eigenfunctions $\psi_n(x)$ corresponding to each energy eigenvalue E_n. Each eigenfunction of the periodic potential is a superposition of box modes $\varphi_m(x)$ according to Eq. (4), where the coefficients c_m are obtained from the eignevectors of the Hamiltonian matrix H.

(a) Building on your MATLAB code from the previous subsection extend the code to evaluate the eigenfunctions $\psi_n(x)$ versus $x = [0, 10]$ using $n_x = 10000$ points.

(b) Plot the eigenfunctions $\psi_n(x)$ versus x for $n = 1, 9, 10, 16$, and superpose the box modes $\varphi_n(x) = 0.6 \sin(k_n x)$ on each plot as a dotted line. You should reproduce the results shown in Fig. 3 of

Ref. [1]. (Hint: Make sure that $\psi_n(x)$ and $\varphi_n(x)$ have the same sign at points where they have similar magnitude. Since eigenfunctions are only determined up to a constant you can always multiply by -1 if need be.)

Your plots illustrate what are called *Bloch standing waves* [1, 2]. The Bloch theorem from your solid state class states that the eigenstates for the periodic lattice may be expressed in the extended zone scheme as $e^{ikx}u_k(x)$, where k is chosen to yield a traveling plane-wave that obeys the periodic boundary conditions, and $u_k(x)$ is a Bloch wave that is a function with the periodicity of the lattice. But here we use box boundary conditions as opposed to periodic boundary conditions, which leads to Bloch standing waves of the form $\phi_n(x) \propto u_n(x)\sin(k_n x)$. Your plots show that the standing wave $\sin(k_n x)$ does indeed act as an envelope that modulates the eigenfunctions [1, 2] in analogy to the traveling plane-waves in the usual Bloch theorem.

D. Tight-binding limit

The example you have been exploring is actually in the so-called *tight-binding limit* that is now elucidated.

(a) Plot the probability density $|\psi_1(x)|^2$ versus $x = [0, 10]$ for the ground state. You should see that the ground state probability is comprised of $(n_b - 1) = 9$ similar localized functions with peaks at integer values of x, which correspond to the centers of the potential wells. In this tight-binding limit the electron wavefunction may be approximated as a superposition of localized functions of differing heights, one around each well.

The individual localized peaks though similar are not independent. To simulate this take the initial condition

$$\Psi(x, 0) = \sqrt{2}e^{-6.25(x-5)^2}, \tag{7}$$

which approximates a particle localized in the central well. You need to resolve this initial wavefunction into the modes of the periodic potential

$$\Psi(x, 0) = \sum_{p=1}^{N} d_p \psi_p(x), \tag{8}$$

where

$$d_p = \int_0^L dx\ \psi_p^*(x)\Psi(x, 0). \tag{9}$$

(b) Using the above information in conjunction with your previous MATLAB solver for the eigenfunctions and eigenvalues of the periodic potential, develop a MATLAB code that can track the evolution of the time-dependent wavefunction $\Psi(x, t)$. With this code produce a plot of the probability density $|\Psi(x, t)|^2$ versus x (vertical axis) and t (horizontal axis) using the MATLAB function `imagesc`. For time take the interval $t = [0, 2]$ using 500 points. (Hint: In the units used here $\hbar = 1$.)

Your simulation should demonstrate that if the wavefunction is initially localized in one potential well it will flow out into the others through the process of quantum tunneling between adjacent wells.

Further exploration: The focus here was on the Krönig-Penny model but the numerical method can be easily extended to other forms of potential [2]. Other topics related to periodic potentials can also be studied, such as surface states, introduction of impurities, and also addition of an external field [1].

[1] F. Le Vot, J. J. Melendez, and S. B. Yuste, "Numerical matrix method for quantum periodic potentials," *Am. J. Phys* **84**, 426 (2016). `https://aapt.scitation.org/doi/abs/10.1119/1.4944706?journalCode=ajp`

[2] R. L. Pavelich and F. Marsiglio, "The Krönig-Penny model extended to arbitrary potentials via numerical matrix mechanics," *Am. J. Phys* **84**, 426 (2015). `https://aapt.scitation.org/doi/10.1119/1.4923026`