Chapter 6 - Problem 1

6.1 The potential energy in a periodic 1D lattice is given by:

$$V(x) = \sum \lambda\, \delta(x - nL)$$

Use the expression previously derived in Chap V for the delta gap transfer matrix to find the forbidden bands for an electron in the interval $0 \le \varepsilon \le 10\, eV$.

Let $\lambda = 0.3$ eV. nm and $L = 0.4$ nm.

In[ ]:=
```
Clear["Global`*"];
```

So first we need our constants, along with our PP-PI matrix functions

Part I. Declare the constants and functions we will use.

PI-PP matrix functions

In[ ]:=
```
Clear["Global`*"];
PI[kL_, kR_] = MatrixExp[(1/2) * Log[kL/kR] * (PauliMatrix[1] - IdentityMatrix[2])];
PP [kx_, l_] = MatrixExp[-I * kx * l * PauliMatrix[3]];
```

Constants (we’ll always use these numbers)

In[ ]:=
```
h = 6.62607004 * 10^(-34) ;(* planck's constant *)
m = 9.10938 * 10^(-31); (* planck's constant *)
ℏ = h/(2 * Pi);
```

Conversion factors:

In[ ]:=
```
e = 1.60217 * 10 ^(-19); (* 1 electron volt (ev) = e Joules *)
nano = 1 * 10^(-9);
```

Given information and other constants/functions:

In[ ]:=
```
λ = 0.3;
L = 0.4;
alpha = Sqrt[(2 * m * e)/ℏ^2] * nano; (* the e and nano will help convert everything at once.*)
k = alpha * Sqrt[epi];
kdelta = alpha * Sqrt[epi - λ/a];
numofbarriers = 1; (* This is artbitrary as long as
 we keep this constant throughout all the subsequent problems *)
```

Part II. Get the Transfer Matrix

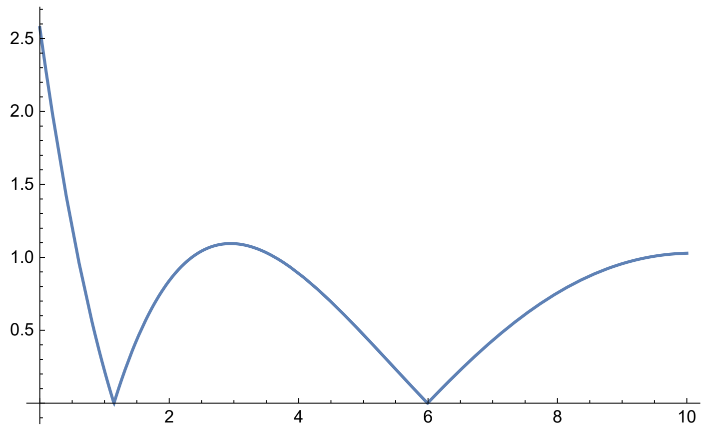
The transfer matrix in this case is made up of PP.PI.PP.and one more PI. Raised to the matrix power of 3 (because we chose 3 to be our number of barriers). You can see above that we set this to a variable that can be changed if we decide that 3 is too many (or too few).

In[ ]:=
```
TransferMatrix = PI[k, kdelta].PP[kdelta, a].PI[kdelta, k].PP[k, L];
```

Now we can use MatrixPower, and since we are using delta approximation then we have to take the Limit as "a" approaches 0. Because a delta function has a width of 0. Then plot.

In[ ]:=
```
TransferMatrix = Limit[MatrixPower[TransferMatrix, numofbarriers](*.PP[k,L]*), a → 0];
TransferPlot = Plot[Abs[Tr[TransferMatrix] / (2)], {epi, 0, 10}]
```

Out[ ]=



Part III. Finding the Forbidden Zone

Okay so to find the find the forbidden bands, we need this :

1. Plot $\left|\frac{1}{2}\text{Tr[TransferMatrix]}\right|$ with respect to energy -> we just did this
2. Let's call this P[[1, 1]] -> this is what he calls it in this notes
3. Then on Chapter 5 Page 6,

this value must satisfy the following equation to be allowed. $|P_{11}| <= 1$

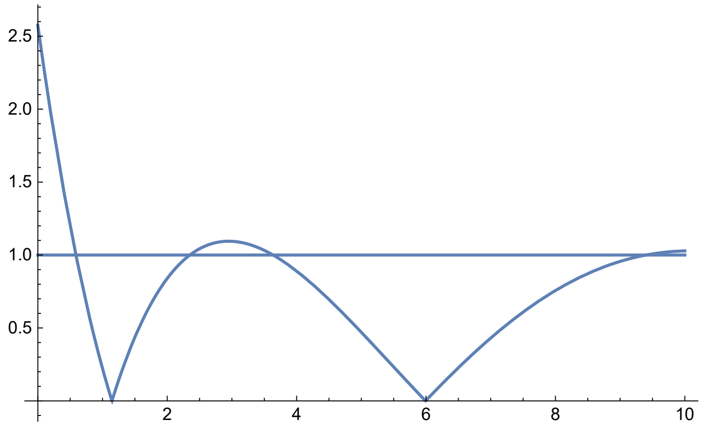
4. In other words, the forbidden zone is located when this condition is NOT satisfied. That is ...

the energy is forbidden if : $|P_{11}| > 1$.

Okay so let's get these forbidden bands ...

In[∘]:=
```
lineatone = Plot[1, {epi, 0, 10}];
Show[TransferPlot, lineatone]
```

Out[∘]=



Okay so we can clearly see the the forbidden bands now. We can use FindRoot to find this because you can find when f(x) == 1 using FindRoot as well. Let’s try it along with the for loop method that we tried in problem 5.7.

```
(* Try to find one root *)
```

In[∘]:=
```
P11 = Tr[TransferMatrix / 2];
FindRoot[Abs[P11] == 1, {epi, 2.2}]
```

Out[∘]=
```
{epi → 2.3502}
```

In[∘]:=
```
(* Okay our test worked, so let's use the for loop method *)
NumOfRoots = 2;
Array[ForbiddenRoots, NumOfRoots ]; (* Results *)
Array[StartSearch, NumOfRoots , 1]; (* where to search *)
StartSearch[1] = 2.2;
StartSearch[2] = 2.5;
 For[i = 1 , i <= NumOfRoots , i++,
  ForbiddenRoots[i] = epi /. FindRoot[Abs[P11] == 1, {epi, StartSearch[i]}];]
For[i = 1, i <= NumOfRoots , i += 2,
 Print["Forbidden band from \n\t",
  ForbiddenRoots[i], " eV to ", ForbiddenRoots[i + 1], " eV"]]
```

```
Forbidden band from
	2.3502 eV to 2.3502 eV
```

Note: If you increase the number of barriers you use, this forbidden band <u>will not change</u>

The first and last roots aren’t within the bounds of 0 - 10 eV, thus we won’t look at them. Within the given the range, there are 3 forbidden bands listed above.

Below is Chapter 6 page 5, which shows what the condition needs to be to be considered a forbidden band.

$|Re(P_{11})| \leq 1 \Rightarrow |\frac{1}{2} tr(P)| \leq 1$ since $P_{11} = P^*_{22}$

this implies that if were to plot $R_e(P_{11})$ as function of energy, there will be regions where the condition is satisfied, these regions are called
allowed bands
and there are regions where the condition is not satisfied and these regions are called forbidden bands.

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