Ex1642: The Kronig Penny model

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The problem:

1. Write the S matrix for a particle scattered by a potential $V(x) = \delta(x)U$.
2. Write the M matrix for the same problem.
   Guidance: the M matrix is a reformulation of the S matrix, only instead of representing the relation between the incoming and outgoing channels, it represents the relation between the left channels and right channels and vise-versa
3. Generalize your answer to the case of N scatterers with a given distance a between them, and receive a transcendental equation for the energy bands.
4. We will define each delta segment as a unit cell. Introducing an asymmetric feature to the system, we now have the $N/2 - 1/2$ unit cell separated a distance b from the $N/2 + 1/2$ unit cell. what is the equation for the eigenenergies of a bounded particle in the b segment?
   What is the minimal b that allows a bound state below the first conduction band?

   Tip: it might be useful to define M as product of "M for delta" and "M for segment". The unit cell can be chosen in asymmetric way, per convenience.

The solution:

1. On both sides of the delta function, the wave function for the particle is:

$$\begin{aligned}\Psi(x<0) = &\quad A_L e^{-ikx} + B_L e^{ikx}\\ \Psi(x>0) = &\quad A_R e^{-ikx} + B_R e^{ikx}\end{aligned}$$

   We will define two channels for a delta potential $V(x) = U\delta(x)$.
   The appropriate S matrix is:

$$S = e^{i\gamma}\begin{pmatrix}\sqrt{g} & -i\sqrt{1-g}\\ -i\sqrt{1-g} & \sqrt{g}\end{pmatrix}$$

$$\begin{aligned}v_E &= \sqrt{2E/m}\\ \gamma(E) &= -\arctan\frac{U}{v_E}\\ g &= \frac{1}{(1+(\frac{U}{v_E})^2)}\\ k &= mv_E\\ u &= mU/k\end{aligned}$$

   Substituting this into the S matrix

$$S = \begin{pmatrix}\frac{-iu}{1-iu} & 1\\ 1 & \frac{-iu}{1-iu}\end{pmatrix}$$

2. The M matrix can be easily deduced from the following relations:

$$\begin{pmatrix}A_L\\ B_L\end{pmatrix} = \begin{pmatrix}M_{11} & M_{12}\\ M_{21} & M_{22}\end{pmatrix}\begin{pmatrix}A_R\\ B_R\end{pmatrix}$$

$$\begin{pmatrix}A_L\\ B_R\end{pmatrix} = \begin{pmatrix}S_{11} & S_{12}\\ S_{21} & S_{22}\end{pmatrix}\begin{pmatrix}A_R\\ B_L\end{pmatrix}$$

   By comparing the M matrix elements to the S matrix elements, we receive:

$$\text{M=}\begin{pmatrix}S_{21} - \frac{S_{22}S_{11}}{S_{12}} & \frac{S_{22}}{S_{12}}\\ \frac{-S_{11}}{S_{12}} & \frac{1}{S_{12}}\end{pmatrix} = \begin{pmatrix}1-iu & -iu\\ iu & 1+iu\end{pmatrix}$$

3. To consider the case of N barriers separated by a length a, will define a transfer matrix T, such that:

$$\begin{pmatrix}A_L\\ B_L\end{pmatrix} = \begin{pmatrix}M_{11} & M_{12}\\ M_{21} & M_{22}\end{pmatrix}\begin{pmatrix}A_R e^{-ika}\\ B_R e^{ika}\end{pmatrix} = MT\begin{pmatrix}A_R\\ B_R\end{pmatrix}$$

$T = \begin{pmatrix} e^{-ika} & 0 \\ 0 & e^{ika} \end{pmatrix}$

So we will redefine our M matrix:

$\mathcal{M} = MT = \begin{pmatrix} e^{-ika} & -iue^{ika} \\ iue^{-ika} & (1+iu)e^{ika} \end{pmatrix}$

So we obtain the connection:

$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = (\mathcal{M})^n \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}$

We could perform this calculation by diagonalizing $\mathcal{M}$
$(\mathcal{M})^n = Q^\dagger D^n Q$
The eigenvalues of $\mathcal{M}$ are $P_\pm = 0.5[tr[\mathcal{M}] \pm \sqrt{tr[\mathcal{M}]^2 - 4}]$

and $tr(\mathcal{M}) = 2(cos(ka) + usin(ka))$

As $|\mathcal{M}| = 1$ we can define $P_\pm = e^{\pm i\lambda}$ and $cos(\lambda) = cos(ka) + usin(ka)$.
Thus our allowed energies are defined by the transcendental equation:

$$|cos(ka) + \frac{2mu}{k}sin(ka)| \leq 1$$

We choose $m = 0.01, u = 100, a = 1$ and graph using desmos for $F(k)$ to show the values of k for which we have allowed energies:

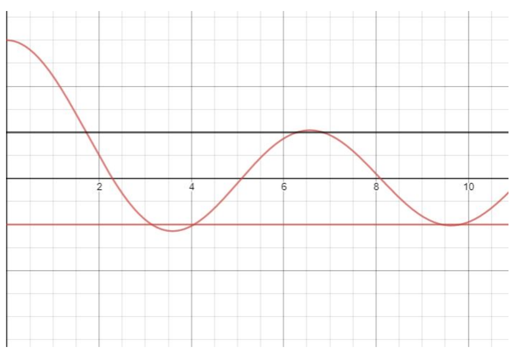

Figure 1: F(k) vs k

We can see that for a delta function we get an infinite series of bands, as expected.

4. After adding a new segment of length b we consider a well potential with length b. We will first show the naive approach, which does give an upper bound for b, but is not the smallest bound possible:

$$E_n^b = \frac{\pi^2 n^2}{2mb^2}$$
$$k_n^b = \frac{\pi n}{b}$$

We substitute the value k_n^b into the transcendental equation from the previous section, to get the allowed energies as a function of b

$$|cos(\frac{\pi na}{b}) + \frac{2mbu}{\pi n}sin(\frac{\pi na}{b})| \leq 1$$

For the case a=b , we get the same bands as above.
For the case$b > a$, we look for the minimal value of b that gives us a bound state, meaning b doesn't fulfill the transcendental equation.
Graphing with the values m=0.01 u=100 and a=1 we get the F(b)-b diagram:

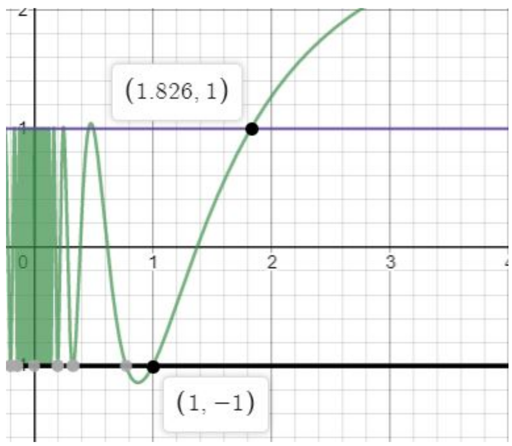

Figure 2: F(b) vs b

We can see that the at b=a=1 we enter an allowed area, and the minimal value of b is $b = 1.826$ with these parameters.

We now provide the more complex but accurate calculation and approach: We are interested for solutions that correspond to the following relation

$$\begin{pmatrix} A_R * e^{-\alpha a} \\ B_R * e^{-\alpha a} \end{pmatrix} = M \begin{pmatrix} A_R \\ B_R \end{pmatrix}$$

Its easy to see that under this scheme $e^{-\alpha a}$ is an eigenvalue of M. Meaning that we can get the value for α by solving for $|det(M - Ie^{-\alpha a})| = 0$
This gives:

$$\alpha = \frac{1}{a} \cosh^{-1}(Tr(M))$$

Now that we have the diminishing factor for the amplitude of the transitioning wave-function, We will demand that $\psi(b/2 + a) = \psi(b/2 + 2a)$. This gives:

$$Acos(k(b/2 + a)) = e^{-\alpha a} Acos(k(b/2 + 2a))$$

Using trigonometric identities, and the fact that $k = \pi/b$ we get that,:

$$2cos(ka) = e^{\alpha a}$$

Plotting for the right and left side, we can see that the right side abruptly ends when $Tr(M) = 1$, we'll define the appropriate k as k_1.
The left side is just a regular cos function, where 1/b determines the width of each wave, so it is enough to choose b such that the value k_b will pass intersect the right side almost twice.
Numerically graphing in desmos we got the following graph:

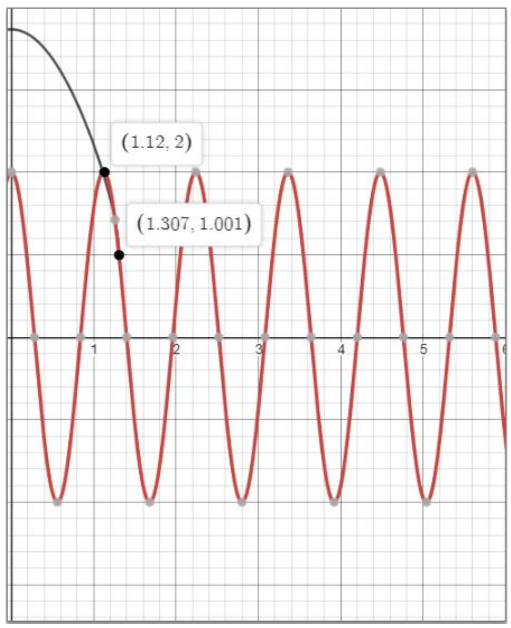

Figure 3: e^{α} vs. $cos(ka)$, m=0.01 u=100 and a=1 b=0.56a