PH3203: Advanced Quantum Mechanics

Scattering from Dirac Comb

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1 Dirac Potential

The Dirac Delta function can be used to model interactions with a localised potential. It can be used to model different aspects of band theory of metals. Here we consider a series of Dirac delta potentials which can be thought to be placed a the lattice sites in metals. We weill consider the scattering amplitutde for a plane wave incident on a series of Dirac delta potentials.

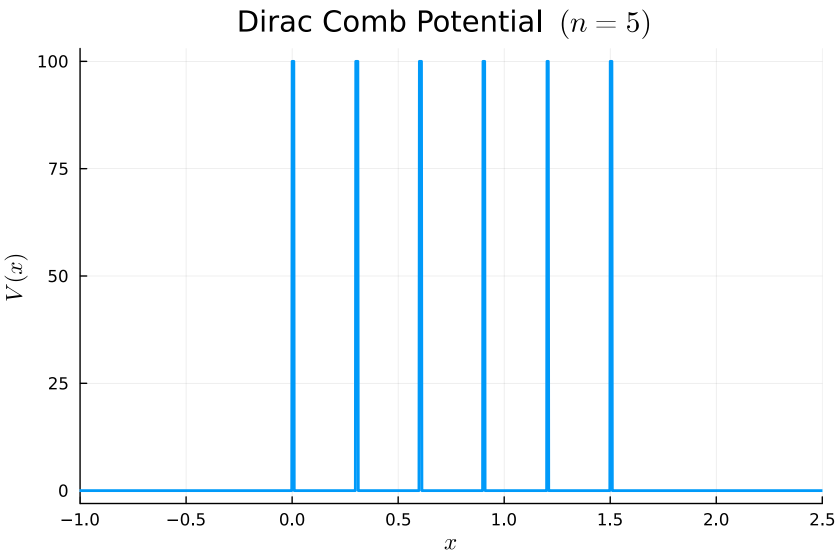

Figure 1: Dirac Comb potential, consisting of five delta potentials. The potential is zero everywhere except at the lattice sites, where it is infinite. Since while plotting, we could not make the potential infinite, we used a sum of square waves with negligible width and appreciable height. This is more like the Kronig-Penney Model.

2 Derivation of Transfer Matrix

Our potential is of the form:

$$\mathrm{V}(x) = \lambda \sum_{n=1}^{N} \delta(x - na)$$

where $\lambda > 0$.
Initially, consider the case of a single Dirac delta potential located at $x = na$. The Schrödinger equation for the particle getting scattered from this potential is given by:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \lambda\delta(x - na)\right)\psi(x) = E\psi(x)$$

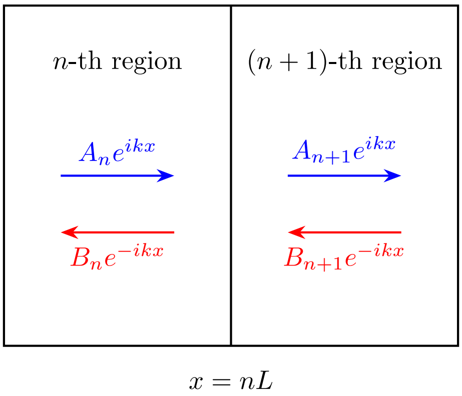

Figure 2: Figure showing scattering from the n^{th} region.

Let the wavefunction in the n^{th} region be given by:

$$\psi(x) = \begin{cases} A_n e^{ikx} + B_n e^{-ikx} & \text{for } x < na \\ A_{n+1} e^{ikx} + B_{n+1} e^{-ikx} & \text{for } x > na \end{cases}$$

where $k = \frac{\sqrt{2mE}}{\hbar}$. Upon imposing the continuity of the wavefunction at $x = na$, we get

$$A_n e^{ikna} + B_n e^{-ikna} = A_{n+1} e^{ikna} + B_{n+1} e^{-ikna}$$

On the other hand, the discontinuity of the derivative of the wavefunction at $x = na$ (due to presence of the delta function) gives us:

$$\left.\frac{d\psi}{dx}\right|_{na^+} - \left.\frac{d\psi}{dx}\right|_{na^-} = \frac{2m\lambda}{\hbar^2}\psi(na)$$
$$\implies ik(A_{n+1}e^{ikna} - B_{n+1}e^{-ikna}) - ik(A_n e^{ikna} - B_n e^{-ikna}) = \frac{2m\lambda}{\hbar^2}(A_n e^{ikna} + B_n e^{-ikna})$$
$$\implies \alpha(A_{n+1}e^{ikna} - B_{n+1}e^{-ikna}) - \alpha(A_n e^{ikna} - B_n e^{-ikna}) = \alpha(A_n e^{ikna} + B_n e^{-ikna})$$

Thus, finally we obtain:

$$\boxed{(1+\alpha)(A_n e^{ikna}) + (1-\alpha)(B_n e^{-ikna}) = \alpha(A_{n+1}e^{ikna} - B_n e^{-ikna})}$$

where $\alpha = \frac{2m\lambda}{\hbar^2 ik}$.

Taking $K = e^{ika}$, the above equations can be written in the form of a matrix equation as:

$$\begin{pmatrix} K^n & K^{-n} \\ (1+\alpha)K^n & (1-\alpha)K^{-n} \end{pmatrix} \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \begin{pmatrix} K^n & K^{-n} \\ \alpha K^n & -\alpha K^{-n} \end{pmatrix} \begin{pmatrix} (1+\alpha)A_n \\ (1-\alpha)B_n \end{pmatrix}$$

Equivalently, this may be written as

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \frac{1}{2\alpha} \begin{pmatrix} 2\alpha - 1 & -K^{-2n} \\ K^{2n} & 2\alpha + 1 \end{pmatrix} \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix}$$

If we use the following transformation,

$$\widetilde{A}_n = A_n K^n \quad \widetilde{B}_n = B_n K^n$$

The transfer matrrix $\mathbf{T}$ between the two states is given by

$$\begin{pmatrix} \widetilde{A}_n \\ \widetilde{B}_n \end{pmatrix} = \frac{\mathbf{T}}{2\alpha} \begin{pmatrix} \widetilde{A}_{n+1} \\ \widetilde{B}_{n+1} \end{pmatrix}$$

where the transfer matrix $\mathbf{T}$ is given by

$$\mathbf{T} = \begin{pmatrix} (2\alpha - 1)K^{-1} & -K \\ K^{-1} & (2\alpha + 1)K \end{pmatrix}$$

It is worth noticing that the transfer matrix $\mathbf{T}$ is a function of k and α but is independent of n, the position of the delta potential.

Now, we focus back to our original problem of N Dirac-delta potentials. Consequently, the system has been divided into $N + 1$ regions, each having a Transmission and reflection coefficient. If we assume that there is no reflection from the rightmost region as there is no barrier present there, the term $\widetilde{B}_{n+1}$ will be zero.

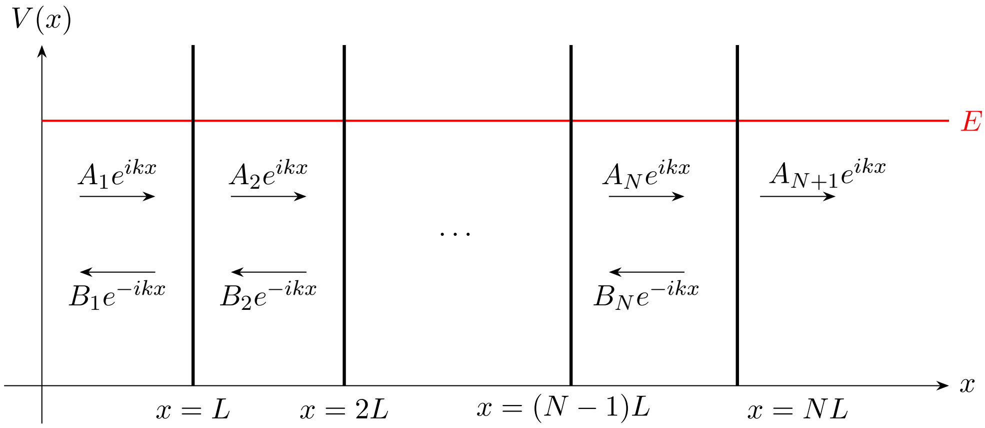

Figure 3: Scattering from multiple regions of the Dirac Comb, depicting the transmissions and reflections.

Our goal will now be to find some relation between the rest $2N + 1$ coefficients. For each of the potentials, the ansatz and the boundary conditions remain the same, hence we may use our results derived in the previous section.
For the first barrier,

$$\begin{pmatrix} \widetilde{A}_1 \\ \widetilde{B}_1 \end{pmatrix} = \frac{1}{2\alpha} \begin{pmatrix} (2\alpha - 1)K^{-1} & -K \\ K^{-1} & (2\alpha + 1)K \end{pmatrix} \begin{pmatrix} \widetilde{A}_2 \\ \widetilde{B}_2 \end{pmatrix}$$

Similarly, for the second potential,

$$\begin{pmatrix} \widetilde{A}_2 \\ \widetilde{B}_2 \end{pmatrix} = \frac{1}{2\alpha} \begin{pmatrix} (2\alpha - 1)K^{-1} & -K \\ K^{-1} & (2\alpha + 1)K \end{pmatrix} \begin{pmatrix} \widetilde{A}_3 \\ \widetilde{B}_3 \end{pmatrix}$$
$$\implies \begin{pmatrix} \widetilde{A}_1 \\ \widetilde{B}_1 \end{pmatrix} = \frac{1}{4\alpha^2} \begin{pmatrix} (2\alpha - 1)K^{-1} & -K \\ K^{-1} & (2\alpha + 1)K \end{pmatrix}^2 \begin{pmatrix} \widetilde{A}_3 \\ \widetilde{B}_3 \end{pmatrix}$$

Here we have exploited the fact that the transfer matrix is independent of n. Note that for the $(N+1)^{\text{th}}$ region, there is only transmission as the initial incident wave is entirely from the right. Thus, we set $\widetilde{B}_{n+1} = 0$. Extending this to N potentials, we get:

$$\begin{pmatrix} \widetilde{A}_1 \\ \widetilde{B}_1 \end{pmatrix} = \left(\frac{\mathbf{T}}{2\alpha} \right)^N \begin{pmatrix} \widetilde{A}_{N+1} \\ 0 \end{pmatrix}$$

Thus, the total transfer matrix is the product of individual transfer matrices of each region. For convenience, we will denote the transfer matrix as $\mathbf{T}^n$ as $\mathbf{M}^{(n)}$. Then, from above we will have:

$$\widetilde{A}_1 = \frac{1}{(2\alpha)^N} \, \mathrm{M}_{11}^{(N)} \widetilde{A}_{N+1}$$

The final transmission probability is given by:

$$\boxed{T_N = \frac{|A_{N+1}|^2}{|A_1|^2} = \frac{|\widetilde{A}_{N+1}|^2}{|\widetilde{A}_1|^2} = \frac{4|\alpha|^{2N}}{\left|\mathrm{M}_{11}^{(N)}\right|^2} = \left(\frac{k\hbar^2}{\lambda m} \right)^{2N} \frac{1}{\left|\mathrm{M}_{11}^{(N)}\right|^2}}$$

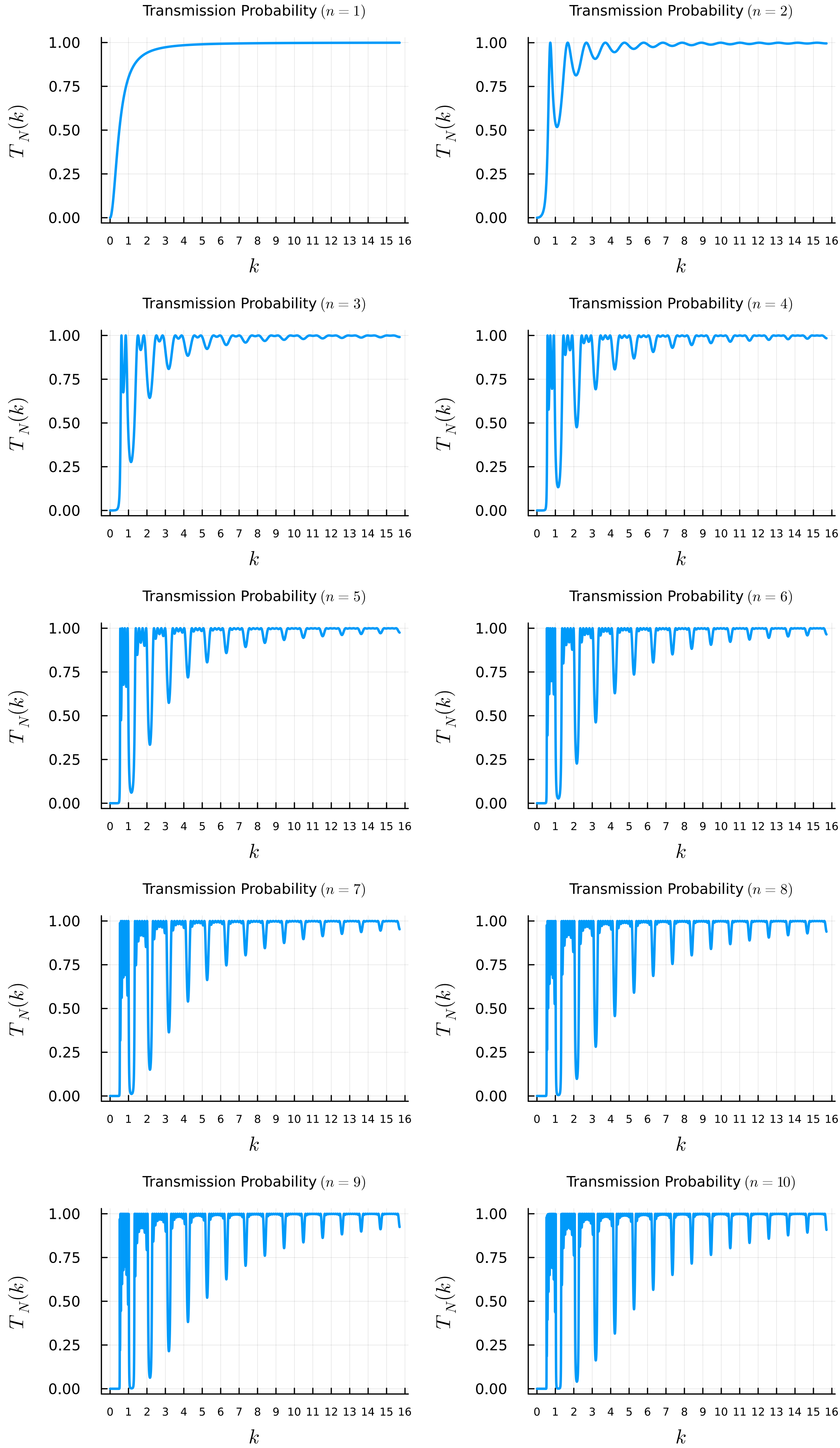

Figure 4: Variation of Transmission Amplitude with k for different number of Dirac-Delta potentials

We numerically computed the variation of transmission probabiltiy with k using the transfer matrix above. We can see that as the number of delta potentials are increased, the tranmission probability shows gapped behaviour. So, there are certain values of k for which the transmission probability is close to zero. This is similar to the band gaps that is formed in metals which makes sense since the Dirac comb can be used to model the localised potentials at the lattice sites of the metal.

The Julia code used to plot the Transmission probability against k is as follows:

```julia
using LinearAlgebra, LaTeXStrings, Plots

n = 10 #number of delta potentials
l = 1

#defining the single transfer matrix
Transfer_Matrix(K, c) = Complex.([
    (2*c - 1)/K -K;
    1/K (2*c + 1)*K
])

#defining the transmission probability using the above derived formula
Trans_prob(k, c, n, L) = ((2*k)^(2*n)) / abs((Transfer_Matrix(exp(1im*k*L), c)^n)[1, 1])

#specifying the range of momentum
k = LinRange(0, 3*pi*l, 10000)
T = zeros(ComplexF64, length(k))

#function which returns the plot of the transmission probability with k for different values of n
function ret_plot(k, n, l)
    for i in eachindex(k)
        T[i] = Trans_prob(k[i], 1im*k[i], n, l)
    end
    return plot(
        k, real.(T),
        xlabel = L"k",
        ylabel = L"T_N(k)",
        title = L"Transmission Probability $(n=%$n)$",
        lw = 2,
        label = "",
        xticks = 0:16,
        titlefontsize = 8,
        titlefont = "sans-serif",
        xtickfontsize = 6
    )
end
A= [ret_plot(k, i, 3.0) for i in 1:10]
plot(A..., layout=(5,2), size=(700,1200), legend=false, left_margin=8Plots.mm)
savefig("T_dirac_1.svg")
```

References

[1] Joaquín Figueroa, Ivan Gonzalez, and Daniel Salinas-Arizmendi. "A Novel Transfer Matrix Framework for Multiple Dirac Delta Potentials". In: (2025). arXiv: 2503.23134 [quant-ph]. URL: https://arxiv.org/abs/2503.23134.