# PHYS20161 $2^{\text{nd}}$ project: Thickness of Boron nitride (BN)

November 5, 2019

BN is a crystalline compound that is composed of 2D layers of boron and nitrogen in a hexagonal lattice. It is often used as an electrical insulator or as a substrate for graphene.

In this project you will measure the thickness of a sample of BN by analysing the fraction of electrons that tunnel through. You will do this using an approach that is very similar to what is implemented at research level.

## 1 Background theory

Quantum tunnelling allows a particle to pass through a potential at energies that classically would be forbidden. The fraction of projectiles that tunnel through the barrier are given by the transmission coefficient, $T$:

$$T = e^{-\beta d}, \tag{1}$$

where $d$ is the thickness of the material and

$$\beta = 2\sqrt{\frac{2m}{\hbar^2}(V_0 - E)}, \tag{2}$$

where the particle has mass $m$ and energy ,$E$. $V_0$ is the height of the potential. this is illustrated in figure 1. Last year you explored QM tunnelling across a square barrier using equation 2 in vibrations and waves (PHYS10302).

In a more realistic scenario, we would expect the barrier to have rounded edges. Therefore the height of the potential varies with distance. This means we instead must integrate over the thickness of the material,

$$T = \exp\left[-2\int_{d_1}^{d_2}\sqrt{\frac{2m}{\hbar^2}(V(x) - E)}dx\right], \tag{3}$$

where $d_2$ and $d_1$ represent the edges of the barrier. For a square well we would find $d_2 - d_1 = d$ from before.

We use the following form for the potential[1],

$$V(x) = V_0 - \frac{1.15\lambda d^2}{x(d-x)}, \tag{4}$$

where

$$\lambda = \frac{e^2 \ln 2}{8\pi\epsilon_r\epsilon_0 d}, \tag{5}$$

[1] We use the same approach as described by Simmons, J. G. (1963). *Generalized formula for the electric tunnel effect between similar electrodes separated by a thin insulating film.* Journal of applied physics, 34(6), 1793-1803.

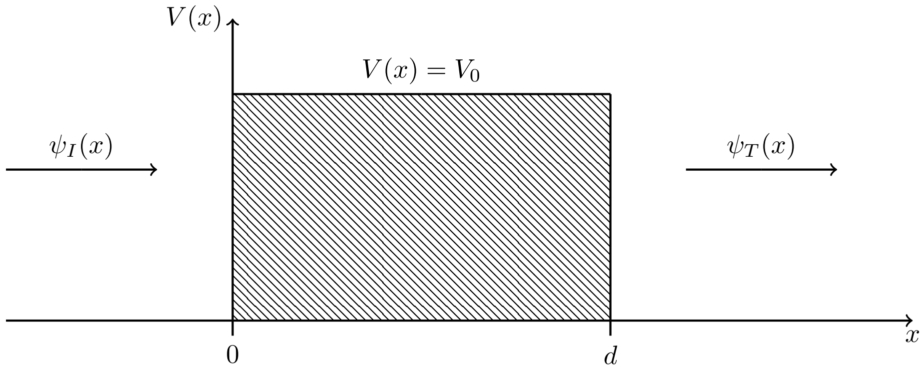


Figure 1: Schematic of an incident wavefunction, $\psi_I(x)$, QM tunnelling across a square barrier to produce a transmitted wavefunction, $\psi_T(x)$, on the other side. The reflected wavefunction has been omitted.

where $\epsilon_r$ is the relative electric permittivity of the material which the electrons are tunnelling across and the rest have their usual meanings. A diagram for this potential is depicted in figure 2. As the edges of the barrier, $d_1$ & $d_2$, no longer lie at 0 and $d$, and the barrier is symmetrical, we find

$$d_1 = \frac{1.2\lambda d}{V_0} \quad \& \quad d_2 = d - d_1. \tag{6}$$

The integral in eq. 3 can be approximated to

$$T \simeq \exp\left[\frac{-2(d_2 - d_1)(2m)^{1/2}}{\hbar}\sqrt{\bar{V} - E}\right], \tag{7}$$

where $\bar{V}$ is the average potential and given by

$$\begin{aligned} \bar{V} &= \frac{1}{d_2 - d_1}\int_{d_1}^{d_2} V(x)dx \\ &= V_0 - \frac{1.15\lambda d}{d_2 - d_1}\ln\left(\frac{d_2(d - d_1)}{d_1(d - d_2)}\right). \end{aligned} \tag{8}$$

## 2 Project description

An experiment has taken place where electrons were fired at a sample of BN a few Angstroms thick. The fraction of transmitted electrons was measured for varying incoming energies. The data can be found in `Tunnelling_data_BN.csv`. There were some faults in the equipment that led to some data points not being recorded correctly.

Your must write a programme that:

- Reads in and validates the data file for both numerical and physical values.
- Finds the thickness, $d$, of the sample in Å to three decimal places by fitting equation 7 using a minimised $\chi^2$ fit. The reduced $\chi^2$ should also be stated to two decimal places.
- Produces a plot of the fit against the data.

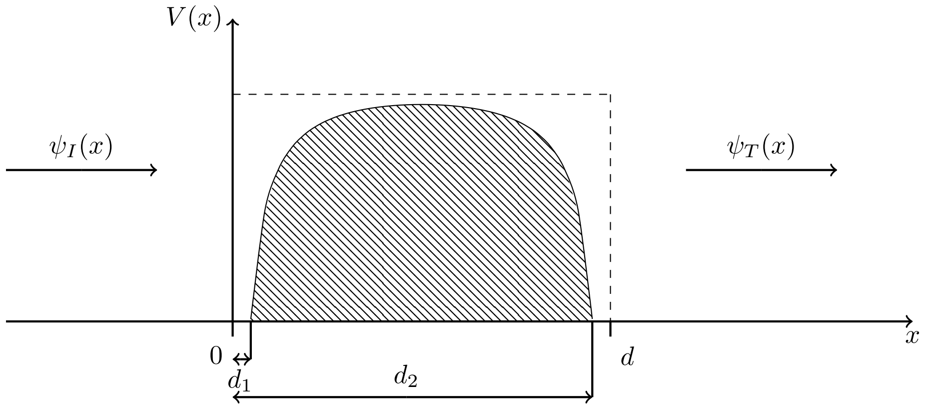


Figure 2: Schematic of an incident wavefunction, $\psi_I(x)$, QM tunnelling across a barrier with round edges to produce a transmitted wavefunction, $\psi_T(x)$, on the other side. $V(x)$ as given in equation 4. The reflected wavefunction has been omitted.

Again we will also be marking you based on style. Further to what was expected in the first assignment, we also expect your code to:

- Be organised.
- Contain a useful check on if the data file exists.
- Produce appropriate plot labels (title and axes).

To achieve this, you may assume that $V_0$ in equation 7 is 3.0 eV and the relative permittivity, $\epsilon$, is 4. You should work in eV and Angstroms ($10^{-10}$ m or Å) throughout. In these units, $\epsilon_0 = 0.00553$ eV / Å (after setting $e$ to 1 eV). In eq. 7 there are a couple of constants that need to be specified in these units. Given the mass of an electron is 0.511 MeV/$c^2$ and $\hbar c = 197.327$ MeV fm, we can write

$$\frac{(2m)^{1/2}}{\hbar} = \frac{(2 \times 0.511\,\text{MeV}\,)^{1/2}}{\hbar c} = \frac{(1.022\,\text{MeV})^{1/2}}{197.327\,\text{MeV fm}} = 0.512317\,\text{eV}^{-1/2}\,\text{Å}^{-1}. \tag{9}$$

The remaining units cancel with the other terms in the exponent.

Additional marks are available for extra features. For instance, can you find the error on the thickness? Given hexagonal BN has layers that are roughly 3 Å thick, how many layers is this sample? Is the code general? Could it be applied to a different data file, *with different validation issues*, and still work correctly? Can you modify your plot beyond the default settings? Can you improve the efficiency of the fitting procedure?

More information on how the mark is split can be found on BlackBoard.