THE QUANTUM WORLD 2021 - 2022
COURSEWORK SET 2

This coursework forms **5%** of your assessment for The Quantum World module.

DEADLINE FOR SUBMISSION: 15:00 on Wednesday Dec. 15.

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1 Scanning tunnelling microscopy (STM) makes it possible to confine electrons in artificial nanostructures. A key example is shown in Fig. 1, where a particle-in-a-box potential has been established via the manipulation of thirty In atoms to form a linear chain. The probability density is shown for each of the three lowest energy eigenstates of this potential well. The experimental data qualitatively agree with the probability densities for the eigenstates of the infinite potential well, $u_n = (\sqrt{2/L})\sin(n\pi x/L)$, where L is the width of the well. In this case $L = 4.45$ nm.

(a) Write a Python program to plot $|u_1(x)|^2$, $|u_2(x)|^2$, and $|u_3(x)|^2$. {**3**}

(b) The wavefunction of an electron in the potential well, $\psi(x)$, can be written in terms of the eigenstates of the Hamiltonian, u_n, as follows:

$$\psi(x) = \sum_n^{\infty} c_n u_n$$

By exploiting the orthonormality of the basis functions u_n, show mathematically that the coefficients c_n are given by the following expression. {**3**}

$$c_n = \int_{-\infty}^{+\infty} u_n^*(x)\psi(x)dx$$

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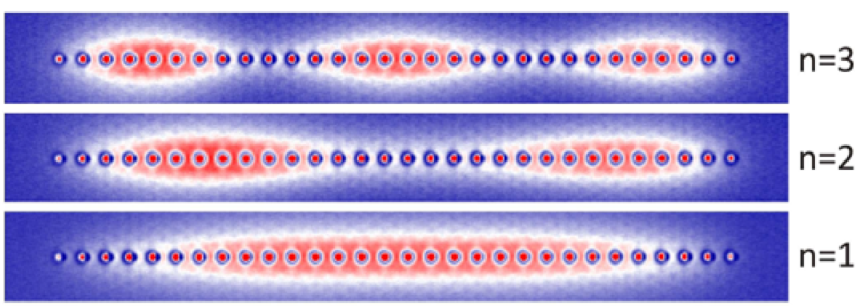

Figure 1: STM images of a thirty-atom chain of In atoms forming a particle-in-a-box confining potential for electrons. The probability density for the $n = 1, n = 2$ and $n = 3$ eigenstates is superimposed on the chain. Remarkably, modelling the confining potential as an infinite potential well provides good agreement with the experimental data. [Taken from *Quantum Rings Engineered by Atom Manipulation*, Van Dong Pham, Kiyoshi Kanisawa, and Stefan Fölsch, *Phys. Rev. Lett.* **123** 066801 (2019)]

At $t = 0$ the system is in the following superposition of the $n = 1$ and $n = 3$ energy eigenstates[1]:

$$\psi(x, t = 0) = \frac{1}{\sqrt{2}} u_1 + \frac{1}{\sqrt{2}} u_3$$

(c) Modify your Python code so that it plots $\psi(x, t = 0)$ $\{\mathbf{2}\}$. Extend your code to numerically determine the values of c_1 and c_3 by calculating the appropriate overlap integrals.$\{\mathbf{4}\}$.

(d) Calculate the energy expectation value, $\langle E \rangle$, for $\psi(x, t = 0)$. Express your answer in eV. $\{\mathbf{2}\}$. (Take $h = 6.626 \times 10^{-34}$ Js and $m = 9.109 \times 10^{-31}$ kg.)

(e) What is the probability of measuring $\langle E \rangle$ as the result of a single measurement of energy at $t = 0$?$\{\mathbf{2}\}$

(f) Write down the expression for $\psi(x, t)\{\mathbf{1}\}$. Hence determine the frequency at which the probability density oscillates.$\{\mathbf{6}\}$

(g) The energy of the particle is found to be E_3 as a result of a single measurement at a time t_1. What energy values will be observed and with what probabilities at a time $t_2 > t_1$?$\{\mathbf{2}\}$

[1] See the *Back In The Box I* interactive figure and TQW Video #21 for a discussion of a superposition state of this type.