University of BRISTOL

(TB1) EENGM0037 - A Quantum Mechanic's Toolbox 2023

Week 1 - 9 Assignments

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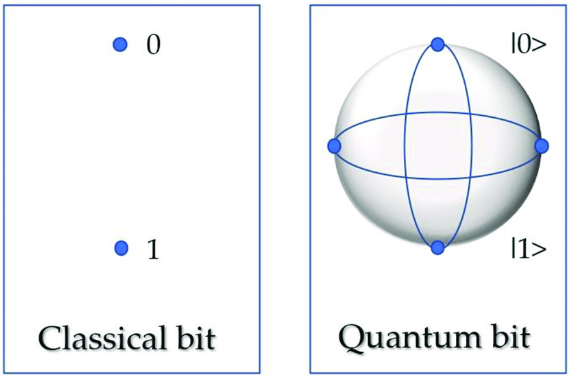
Week 1

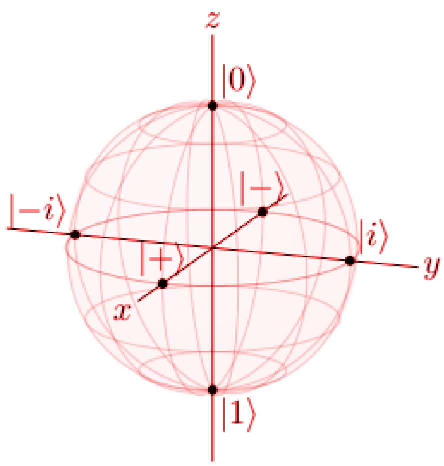
This week's problem sheet contains exercises taken from Introduction to Classical and Quantum Computing by Thomas G. Wong (2021), our course textbook, as well as some other exercises.

1. Write a one sentence definition of a. a bit and b. a qubit. You should include a relevant diagram to explain your answer.



a. A bit is the basic unit of data that a computer can process and store which can have a value either 0 or 1.
b. A qubit is the basic unit of quantum information in quantum computing which can have a value that is either 0, 1 or a quantum superposition of 0 and 1.

2. On a Bloch sphere, illustrate the states: |0>, |1>, |+>, |->, |-i> and |i>



3. Complete exercise 2.8 and 2.9 in Wong

Exercise 2.8. A qubit is in the state

$$\frac{e^{i\pi/8}}{\sqrt{5}}|0\rangle + \beta|1\rangle.$$

What is a possible value of β?

The possible value of β for $\frac{e^{i\pi/8}}{\sqrt{5}}|0 + \beta|1 >$ is calculated below.

$$|\frac{e^{i\pi/8}}{\sqrt{5}}|^2 + |\beta|^2 = 1$$

$$(\frac{e^{i\pi/8}}{\sqrt{5}})(\frac{e^{-i\pi/8}}{\sqrt{5}}) + |\beta|^2 = 1$$

$$|\beta|^2 = 1 - (\frac{(-1)^{1/8}}{\sqrt{5}})(\frac{(-1)^{-1/8}}{\sqrt{5}})$$

$$|\beta|^2 = \frac{4}{5}$$

$$\beta = \pm \frac{2}{\sqrt{5}}$$

Exercise 2.9. A qubit is in the state

$$A\left(2e^{i\pi/6}|0\rangle - 3|1\rangle\right).$$

(a) Normalize the state (i.e., find A).
(b) If you measure the qubit, what is the probability that you get $|0\rangle$?
(c) If you measure the qubit, what is the probability that you get $|1\rangle$?

a. $(|A|\,|2e^{i\pi/6}|)^2 + ((|A|\,|-3|))^2 = 1$

$(2e^{i\pi/6})\ (2e^{-i\pi/6})|A|^2 + 9|A|^2 = 1$

$(2(-1)^{1/6}2(-1)^{-1/6}\ |A|^2 + 9A|A|^2 = 1$

$4|A|^2\ + 9|A|^2 = 1$

$A = \pm \frac{1}{\sqrt{13}}$

b. Probability to get |0> is 4/13.
c. Probability to get |0> is 9/13.

4. Read section 2.3.3 (p86-88 in Wong) and complete exercises 2.10 and 2.11

Exercise 2.10. A qubit is in the state

$$\frac{1}{2}|0\rangle - \frac{\sqrt{3}}{2}|1\rangle.$$

(a) If you measure it in the Z-basis $\{|0\rangle, |1\rangle\}$, what states can you get and with what probabilities?
(b) Write the qubit's state in terms of $|+\rangle$ and $|-\rangle$.
(c) If you measure it in the basis $\{|+\rangle, |-\rangle\}$, what states can you get and with what probabilities?

a. State for qubit measured in Z-basis is $\frac{1}{2}|0> - \frac{\sqrt{3}}{2}|1>$.

Probability of getting 0|> is ¼.

Probability of getting 1> is ¾.

b. Substituting the equations of +|> and -|> into the state of the qubit

$$\frac{1}{2}|0> - \frac{\sqrt{3}}{2}|1> = \frac{1}{2}\frac{1}{\sqrt{2}}(|+> + |->) - \frac{\sqrt{3}}{2}\frac{1}{\sqrt{2}}(|+> - |->)$$

$$= \frac{1-\sqrt{3}}{2\sqrt{2}}|+> + \frac{1+\sqrt{3}}{2\sqrt{2}}|->$$

c. |+> probability is $(\frac{1-\sqrt{3}}{2\sqrt{2}})(\frac{1+\sqrt{3}}{2\sqrt{2}}) = \frac{1-2\sqrt{3}+3}{8} = \frac{2-\sqrt{3}}{4} = 6.7\%$

|-> probability is $(\frac{1+\sqrt{3}}{2\sqrt{2}})(\frac{1+\sqrt{3}}{2\sqrt{2}}) = \frac{2+\sqrt{3}}{4} = 93.3\%$

Exercise 2.11. The following two states are opposite points on the Bloch sphere:

$$|a\rangle = \frac{\sqrt{3}}{2}|0\rangle + \frac{i}{2}|1\rangle,$$
$$|b\rangle = \frac{i}{2}|0\rangle + \frac{\sqrt{3}}{2}|1\rangle.$$

So, we can measure relative to them. Now consider a qubit in the state

$$\frac{1}{2}|0\rangle - \frac{\sqrt{3}}{2}|1\rangle.$$

(a) Write the qubit's state in terms of $|a\rangle$ and $|b\rangle$.
(b) If you measure the qubit in the basis $\{|a\rangle, |b\rangle\}$, what states can you get and with what probabilities?

a. $|0> = \frac{\sqrt{3}}{2}|a> - \frac{i}{2}|b>$, $|1> = \frac{-1}{2}|a> - \frac{\sqrt{3}}{2}|b>$

Substituting, the state of our qubit is

$$\frac{1}{2}|0> - \frac{\sqrt{3}}{2}|1> = \frac{1}{2}(\frac{\sqrt{3}}{2}|a> - \frac{i}{2}|b>) - \frac{\sqrt{3}}{2}(\frac{-i}{2}|a> + \frac{\sqrt{3}}{2}|b>)$$

$$= \frac{\sqrt{3}(1+i)}{4}|a> - \frac{3+i}{4}|b>$$

b. |a> probability is $|\frac{\sqrt{3}(1+i)}{4}|^2 = \frac{3}{8}$

|b> probability is $|-\frac{3+i}{4}|^2 = \frac{5}{8}$

5. Suppose a qubit is in state |0>. You measure it in the Z-basis (|0>, |1>). What outcomes are possible, with what probabilities.

The state remains unchanged. Probability for |0> is 1, for |1> is 0.

6. a. You measure a qubit in the state 1/ √2 (|0> + |1>) in the z-basis. What is the probability of measuring a |0>?

P(|0>) is (1/ √2)^2 = ½.

b. Suppose after the measurement you do, in fact, measure a |0>. If you repeat the measurement in the Z-basis, what is the probability of measuring a |0>?

P(|0>) is still ½.

c. Next, you perform a measurement in the (|+>, |->) basis. What are the possible outcomes, and with what probabilities?

If we measure in the X-basis {|+⟩,|−⟩}, then since both |0⟩ and |1⟩ are halfway between |+⟩ and |−⟩, the qubit collapses to |+⟩ or |−⟩, each with probability ½.

7, 8,9, 10 : Do exercise 2.18 and 2.19 from Wong (below)

Exercise 2.18. A review of various ways to build a quantum computer is the article "Quantum Computers" by Ladd *et al.* (2010). The published version in *Nature* 464, 45–53 is available at https://dx.doi.org/10.1038/nature08812, but it may require a subscription. Search through the text and fill in the blanks:

(a) Photons: "Realizing a qubit as the ________ state of a photon is appealing because photons are relatively free of the ________ that plagues other quantum systems."
(b) Trapped ions: "Individual atomic ions can be confined in free space with nanometre precision using appropriate ________ ________ from nearby electrodes."
(c) Cold atoms: "An array of cold neutral atoms may be confined in free space by a pattern of crossed ________ ________, forming an optical lattice."
(d) Nuclear magnetic resonance: "In a ________, nuclear Larmor frequencies vary from atom to atom [...] Irradiating the nuclei with resonant ________ pulses allows manipulation of nuclei of distinct frequency, giving generic ________ gates."
(e) Quantum dots: "These 'artificial atoms' occur when a small semiconductor nanostructure, impurity or impurity complex binds one or more electrons or holes (empty valence-band states) into a localized potential with ________ ________ ________, which is analogous to an electron bound to an ________ ________."
(f) Doped solids: "________ ________ may then be stored in either the donor electron, or in the state of the single ^{31}P nuclear spin, accessed via the electron-nuclear ________ coupling."
(g) Nitrogen-vacancy centers: "The ________ state of a nitrogen-vacancy centre may then be coherently manipulated with resonant ________ fields, and then detected in a few milliseconds via spin-dependent flourescence in an ________ microscope."
(h) Superconductors: "There are three basic types of superconducting qubits—________, ________ and ________."

a. polarization, decoherence
b. electric field
c. laser beams
d. molecule, radio-frequency, one-qubit
e. discrete energy levels, atomic nucleus
f. quantum information, hyperfine
g. spin, microwave, optical
h. charge, flux, phase

Exercise 2.19. Visit https://en.wikipedia.org/wiki/List_of_companies_involved_in_quantum_computing_or_communication for a list of companies involved in quantum computing. For each of the following types of qubits, name a company that is using them.
(a) Photons
(b) Trapped ions
(c) Cold atoms
(d) Nuclear magnetic resonance (NMR)
(e) Quantum dots
(f) Defect qubits
(g) Superconductors

a. AUREA Technology
b. ionQ
c. ColdQuanta Inc.
d. HP
e. NEC Corporation
f. Quantum Brilliance
g. Amazon

Exercise 2.20. Visit https://qubitzoo.com and pick your favorite qubit.
(a) What is the name of your qubit? (e.g., exchange-only qubit, not Steve.)
(b) What type of technology is your qubit?
(c) What is some motivation for building a qubit this way?

a. Fluxonium
b. Superconducting
c. The fluxonium is an attempt to combine the better features of the type of superconducting charge qubit, named Transmon (insensitivity to charge noise) and flux qubit (strong anharmonicity).

Exercise 2.21. Visit https://en.wikipedia.org/wiki/Qubit#Physical_implementations and pick a qubit.
(a) What is the physical system or technology used for your qubit (physical support)?
(b) What is the name of your type of qubit?
(c) What physical property is used to store information (information support)?
(d) What state is typically used for $|0\rangle$?
(e) What state is typically used for $|1\rangle$?

a. Josephson junction, which can be thought of as an inductor with strong non-linearity and negligible energy loss.
b. Superconducting phase qubit
c. Energy. The phase qubit is operated in the zero-voltage state. At very low temperatures, with a sufficiently high resistance and small capacitance Josephson junction, quantum energy levels become detectable in the local minima of the washboard potential.
d. Ground state
e. First excited state

11: Open an Excel or similar spreadsheet file on your PC. Make a list of quantum related words in there, and write definitions for them.

- Quantum = the smallest discrete unit of a phenomenon. For example, a quantum of light is a photon, and a quantum of electricity is an electron.

- Superposition = quantum phenomena where a particle can exist in two states at the same time.

- Coherence = property of a quantum system that allows it to maintain and preserve the phase relationship between different quantum states.

- Quanum state = described by a complex function Ψ, which depends on the coordinate x and on time: $\Psi(x,t)$. The wave function encodes all the information about the system.

- Bloch sphere = a geometrical representation of the pure state space of a 2-level quantum system. Its purpose is to give a geometric explanation to single-qubit operations.

- Quantum Teleportation = a process that allows the transfer of quantum information from one location to another, without physically transporting the particles themselves. It relies on entanglement and classical communication to faithfully transmit the quantum state from a sender to a receiver.

Week 2

1.

Exercise 2.22. Consider a map U that transforms the Z-basis states as follows:

$$U|0\rangle = |0\rangle + |1\rangle,$$
$$U|1\rangle = |0\rangle - |1\rangle.$$

Say $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ is a normalized quantum state, i.e., $|\alpha|^2 + |\beta|^2 = 1$.

(a) Calculate $U|\psi\rangle$.

(b) From your answer to (a), is U a valid quantum gate? Explain your reasoning.

a. $U|\psi> \;= U\alpha|0> + U\beta|1>$

$U|\psi> \;= \alpha(|0> + |1>) + \beta(|0> - |1>)$

$U|\psi> \;= (\alpha + \beta)|0> + (\alpha - \beta)|1>$

b. $|\alpha + \beta|^2 + |\alpha - \beta|^2$

$= |\alpha^2 + 2\alpha\beta + \beta^2 + \alpha^2 - 2\alpha\beta + \beta^2|$

$= 2|\alpha^2 + \beta^2|$

Since the fact given that $|\alpha|^2 + |\beta|^2 = 1$, therefore the probability is 2 which proves U is an invalid quantum gate.

2.

Exercise 2.23. Consider a map U that transforms the Z-basis states as follows:

$$U|0\rangle = \frac{\sqrt{3}}{2}|0\rangle + \frac{\sqrt{3}+i}{4}|1\rangle,$$
$$U|1\rangle = \frac{\sqrt{3}+i}{4}|0\rangle - \frac{\sqrt{3}+3i}{4}|1\rangle.$$

Say $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ is a normalized quantum state, i.e., $|\alpha|^2 + |\beta|^2 = 1$.

(a) Calculate $U|\psi\rangle$.

(b) From your answer to (a), is U a valid quantum gate? Explain your reasoning.

a. $U|\psi> \;= U\alpha|0> + U\beta|1>$

$U|\psi> \;= \alpha(\frac{\sqrt{3}}{2}|0> + \frac{\sqrt{3}+i}{4}|1>) + \beta(\frac{\sqrt{3}+i}{4}|0> - \frac{\sqrt{3}+3i}{4}|1>)$

$U|\psi> \;= (\frac{\sqrt{3}}{2}\alpha + \frac{\sqrt{3}+i}{4}\beta)|0> + (\frac{\sqrt{3}+i}{4}\alpha + \frac{-\sqrt{3}-3i}{4}\beta)|1>$

b. $|\frac{\sqrt{3}}{2}\alpha + \frac{\sqrt{3}+i}{4}\beta|^2 + |\frac{\sqrt{3}+i}{4}\alpha - \frac{\sqrt{3}+3i}{4}\beta|^2$

$= (\frac{\sqrt{3}}{2}\alpha + \frac{\sqrt{3}+i}{4}\beta)(\frac{\sqrt{3}}{2}\alpha^* + \frac{\sqrt{3}-i}{4}\beta^*) + (\frac{\sqrt{3}+i}{4}\alpha - \frac{\sqrt{3}+3i}{4}\beta)(\frac{\sqrt{3}-i}{4}\alpha^* - \frac{\sqrt{3}-3i}{4}\beta^*)$

$= \frac{12}{16}|\alpha|^2 + (\frac{\sqrt{3}}{2})(\frac{\sqrt{3}+i}{4})\alpha^*\beta + (\frac{\sqrt{3}}{2})(\frac{\sqrt{3}-i}{4})\alpha\beta^* + \frac{4}{16}|\beta|^2$

$+ \frac{4}{16}|\alpha|^2 - (\frac{\sqrt{3}+3i}{4})(\frac{\sqrt{3}-i}{4})\alpha^*\beta - (\frac{\sqrt{3}+i}{4})(\frac{\sqrt{3}-3i}{4})\alpha\beta^* + \frac{12}{16}|\beta|^2$

$= \frac{12}{16}|\alpha|^2 + \frac{12}{8}|\alpha|^2 + \frac{12}{8}|\beta|^2 + \frac{4}{16}|\beta|^2 + \frac{4}{16}|\alpha|^2 - \frac{12}{8}|\alpha|^2 - \frac{12}{8}|\beta|^2 + \frac{12}{16}|\beta|^2$

$= |\alpha|^2 + |\beta|^2$

Since the fact given that $|\alpha|^2 + |\beta|^2 = 1$, therefore the probability is 1 which proves U is a valid quantum gate.

3.

Exercise 2.24. Consider each of the following classical logic gates with input A, output B, and truth table shown below. Is each gate a valid quantum gate? Why?

(a)

A	B
0	0
1	1

(b)

A	B
0	1
1	1

a. Yes, because reversible.
b. No, because irreversible.

4.

Exercise 2.25. Consider each of the following classical logic gates with inputs A and B, outputs C and D, and truth table shown below. Is each gate a valid quantum gate? Why?

(a)

A	B	C	D
0	0	0	1
0	1	1	1
1	0	0	0
1	1	1	0

(b)

A	B	C	D
0	0	0	0
0	1	0	0
1	0	1	0
1	1	1	1

a. Yes, because reversible.
b. No, because irreversible.

5.

Exercise 2.26. Calculate $Z^{217}X^{101}Y^{50}(\alpha|0\rangle + \beta|1\rangle)$.

$Z^{217}X^{101}Y^{50}(\alpha|0>+\beta|1>)$

$= Z\ X\ (\alpha|0>+\beta|1>)$

$= Z(\alpha|1>+\beta|0>)$

$= \beta|0>-\alpha|1>$

6.

Exercise 2.27. Prove that
(a) $XZXZ(\alpha|0\rangle + \beta|1\rangle) = -(\alpha|0\rangle + \beta|1\rangle)$.
(b) $ZXZX(\alpha|0\rangle + \beta|1\rangle) = -(\alpha|0\rangle + \beta|1\rangle)$.

a. $XZXZ(\alpha|0>+\beta|1>)$

$= XZX(\alpha|0>-\beta|1>)$

$= XZ(\alpha|1>-\beta|0>)$

$= X(-\alpha|1>-\beta|0>)$

$= -\alpha|0>-\beta|1>$

$= -(\alpha|0>+\beta|1>)$

b. $ZXZX(\alpha|0>+\beta|1>)$

$= ZXZ(\alpha|1>+\beta|0>)$

$= ZX(-\alpha|1>+\beta|0>)$

$= Z(-\alpha|0>+\beta|1>)$

$= -\alpha|0>-\beta|1>$

$= -(\alpha|0>+\beta|1>)$

7.

Exercise 2.29. Say $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ is a normalized quantum state, i.e., $|\alpha|^2 + |\beta|^2 = 1$.
(a) Calculate $H|\psi\rangle$.
(b) Show that the total probability of $H|\psi\rangle$ is 1, so H is a valid quantum gate.

a. $H|\psi >$

$$= H(\alpha|0 >+ \beta|1 >)$$
$$= \alpha H|0 >+ \beta H|1 >$$
$$= \alpha(\frac{1}{\sqrt{2}}|0 >+ \frac{1}{\sqrt{2}}|1 >) + \beta(\frac{1}{\sqrt{2}}|0 >- \frac{1}{\sqrt{2}}|1 >)$$
$$= \frac{\alpha+\beta}{\sqrt{2}}|0 >+ \frac{\alpha-\beta}{\sqrt{2}}|1 >$$

b. P($H|\psi >$)

$$= |\frac{\alpha+\beta}{\sqrt{2}}|^2 + |\frac{\alpha-\beta}{\sqrt{2}}|^2$$
$$= \frac{|\alpha|^2+2|\alpha||\beta|+|\beta|^2}{2} + \frac{|\alpha|^2-2|\alpha||\beta|+|\beta|^2}{2}$$
$$= \frac{2|\alpha|^2+2|\beta|^2}{2}$$
$$= |\alpha|^2 + |\beta|^2$$
$$= 1$$

8.

Exercise 2.30. Work out the math to show that
(a) $H|-\rangle = |1\rangle$.
(b) $H|-i\rangle = e^{-i\pi/4}|i\rangle \equiv |i\rangle$.

a. $H| ->$

$$= H(\frac{1}{\sqrt{2}}|0 >- \frac{1}{\sqrt{2}}|1 >)$$
$$= \frac{1}{\sqrt{2}}(\frac{1}{\sqrt{2}}|0 >+ \frac{1}{\sqrt{2}}|1 >) - \frac{1}{\sqrt{2}}(\frac{1}{\sqrt{2}}|0 >- \frac{1}{\sqrt{2}}|1 >)$$
$$= \frac{1}{2}|0 >+ \frac{1}{2}|1 >) - \frac{1}{2}|0 >+ \frac{1}{2}|1 >$$
$$= |1 >$$

b. $H| - i >$

$$= \frac{1}{\sqrt{2}}(H|0 >- iH|1 >)$$
$$= \frac{1}{\sqrt{2}}[(\frac{1}{\sqrt{2}}(|0 >+ |1 >) - \frac{i}{\sqrt{2}}(|0 >- |1 >)]$$
$$= \frac{1}{\sqrt{2}}(\frac{1-i}{\sqrt{2}}|0 >+ \frac{1+i}{\sqrt{2}}|1 >)$$
$$= \frac{1}{\sqrt{2}}(cos\frac{\pi}{4} - isin\frac{\pi}{4})|0 >+ (cos\frac{\pi}{4} + isin\frac{\pi}{4})|1 >)$$
$$= \frac{1}{\sqrt{2}}(e^{-i\frac{\pi}{4}}|0 >+ e^{i\frac{\pi}{4}}|1 >)$$
$$= \frac{1}{\sqrt{2}}e^{-i\frac{\pi}{4}}(|0 >+ e^{-i\frac{\pi}{2}}|1 >)$$
$$= \frac{1}{\sqrt{2}}e^{-i\frac{\pi}{4}}(|0 >- i|1 >)$$
$$= e^{-i\frac{\pi}{4}}(- |i >)$$
$$= |i >$$

9. Make your own table of the gates from the lecture, what the result of operating on a qubit with them.

Gate Name	Operation
identity gate	I|0> = |0>
	I|1> = |1>
Pauli X gate (NOT gate)	X|0> = |1>
	X|1> = |0>
Pauli Y gate	Y|0> = i|1>
	Y|1> = -i|0>
Pauli Z gate	Z|0> = |0>
	Z|1> = -|1>
Phase gate	S|0> = |0>
notes: $S^2 = T$	S|1> = i|1>
T gate	T|0> = |0>
notes: $T^2 = S$	$T\|1>= e^{\frac{i\pi}{4}}\|1>$
Hadamard gate	$H\|0>= \frac{1}{\sqrt{2}}(\|0>+\|1>) = \|+>$
	$H\|1>= \frac{1}{\sqrt{2}}(\|0>-\|1>) = \|->$

10. *Update your glossary.* Update your glossary with additional terms from this week, including entanglement, reversible gate, valid gate. You should also add **5 terms** you didn't understand from the paper you read last week, and attempt to define them.

Entanglement

Definition: a phenomenon where two or more quantum particles become interconnected in such a way that the quantum state of one particle is dependent on the state of another, regardless of the physical distance separating them. A product state contains no correlations, while there is a correlation between the entangled qubits, differences explained below.

Product State

Example 1

$\lvert + \rangle$ —	$\lvert +0 \rangle$ —	$\lvert 0 \rangle$

Example 2

$$|a\rangle = \begin{bmatrix} a_0 \\ a_1 \end{bmatrix}, \quad |b\rangle = \begin{bmatrix} b_0 \\ b_1 \end{bmatrix}.$$

$$|ba\rangle = \begin{bmatrix} b_0 a_0 \\ b_0 a_1 \\ b_1 a_0 \\ b_1 a_1 \end{bmatrix}.$$

Entangled State

Example 1

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle).$$

This represents a different kind of two-qubit state, distinct from the product states, which cannot be described as combination of simple single qubit states

Reversible gate

Definition: a logic gate where, given the output(s) of the gate, we can always determine what the input(s) was (were), examples: X gate, Y gate, Z gate, H gate, etc.

Valid gate

A valid quantum gate must be a unitary operator (Unitarity ensures that the quantum gate is reversible) and the total probability must remain 1.

Decoherence

This describes the loss of quantum coherence and the transition from quantum behavior to classical behavior in quantum systems. It occurs when a quantum system, which is initially in a superposition of states, becomes entangled with its surrounding environment (or "bath") and loses its quantum properties.

Spin-qubit

A type of qubit (quantum bit) that is based on the quantum properties of an electron's spin. They rely on the intrinsic angular momentum of electrons, known as spin, to represent and manipulate quantum information.

Quantum dots

A quantum dot is a nanoscale semiconductor structure with unique optical and electronic properties due to quantum confinement effects. Quantum dots are artificially engineered materials and can behave like artificial atoms. They are used in various applications, including displays, biological imaging, and as potential components in quantum computing. Quantum dots are not qubits themselves but can be used as part of a quantum device to manipulate or read out qubits in certain quantum systems.

Optical lattices

Optical lattices are a versatile experimental tool in the field of atomic, molecular, and optical physics, as well as in quantum optics and quantum simulation. They are created by trapping and cooling atoms using lasers and magnetic fields to form a periodic arrangement of potential energy wells. This periodic arrangement mimics the lattice structure found in solid-state crystals but with much greater control and flexibility.

Quantum Error Correction (QEC) protocol

A quantum error correction protocol is a set of procedures and techniques designed to detect and correct errors that naturally occur in quantum computations. Quantum computers are sensitive to errors due to factors like environmental noise, decoherence, and imperfect quantum gates. Example of QEC cdoes include bit-flip, phase-flip, shor code, etc.

Week 3

Glossary

Hermitian conjugate operation

$A^\dagger$ Hermitian conjugate: $\begin{bmatrix} a & c \\ b & d \end{bmatrix}^\dagger = \begin{bmatrix} a^* & b^* \\ c^* & d^* \end{bmatrix}$

$$(aA)^\dagger = a^* A^\dagger$$

$$(A^\dagger)^\dagger = A$$

$$(A+B)^\dagger = A^\dagger + B^\dagger$$

$$(AB)^\dagger = B^\dagger A^\dagger$$

$$(AB|\psi>)^\dagger =< \psi|B^\dagger A^\dagger$$

Ket vector and Bra vector

Ket

The values (a, b and c above) are complex numbers (they may be real numbers, imaginary numbers or a combination of both)
A ket is a quantum state
Kets can have any number of dimensions, including infinite dimensions

E.g. $|a\rangle = \begin{bmatrix} 2-3i \\ 6+4i \\ 3-i \end{bmatrix}$

Bra

The "bra" is similar, but the values are in a row, and each element is the complex conjugate of the ket's elements. The values are not only in a row, but also the sign (+ to −, and − to +) in the middle of each element should be changed.

E.g. $\langle a| = \begin{bmatrix} 2+3i & 6-4i & 3+i \end{bmatrix}$

Inner product / scalar product

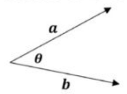
= a generalisation of the dot product. In a vector space, it is a way to multiply vectors together, with the result of this multiplication being a scalar.

Dot Product Formula 1

if $\vec{a} = x_1\vec{i} + y_1\vec{j} + z_1\vec{k}$ and $\vec{b} = x_2\vec{i} + y_2\vec{j} + z_2\vec{k}$

$$a \cdot b = x_1x_2 + y_1y_2 + z_1z_2$$

Dot Product Formula 2



$$a \cdot b = |a||b|cos\theta$$

Normalised

We say a quantum state is normalised if its total probability is 1.

E.g. $$\langle\psi|\psi\rangle = (\alpha^* \ \beta^*)\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = |\alpha|^2 + |\beta|^2 = 1.$$

Orthogonal

Orthogonality is a relation between two states $|\phi\rangle$ and $|\varphi\rangle$. Two such states are orthogonal iff $\langle\phi|\varphi\rangle=0$.

E.g. $$\langle 0|1\rangle = (1 \ 0)\begin{pmatrix}0 \\ 1\end{pmatrix} = 1\cdot 0 + 0\cdot 1 = 0 + 0 = 0.$$

Orthonormal

A set of vectors S is orthonormal if every vector in S has magnitude 1 and the set of vectors are mutually orthogonal.

Orthonormal = normalised + orthogonal

Operators

Operators in quantum mechanics are mathematical entities used to represent physical processes that result in the change of the state vector of the system, such as the evolution of these states with time.

Linear algebra

The branch of mathematics that deals with vectors, matrices, finite or infinite dimensions as well as a linear mapping between such spaces is defined as linear algebra.

Commutator

The commutative law does not generally hold for operators. In general, $\hat{A}\hat{B} \neq \hat{B}\hat{A}$. It is convenient to define the quantity $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$ which is called the commutator of $\hat{A}$ and $\hat{B}$. Note that the order matters, so that $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$.

Eigenvalue and Eigenstate

The eigenvalue equation of an operator $\widehat{O}$ is $\widehat{O}|\rangle = \lambda|x\rangle$ where λ is an unknown number and $|x\rangle$ is an unknown ket. This equation has many solutions $|x_\alpha\rangle$, which are called eigenstates of $\widehat{O}$. For each solution $|x_\alpha\rangle$, there is a number λ_α, called the eigenvalue corresponding to the eigenstates $|x_\alpha\rangle$.

Tensor product

Using the bra-ket notation, the abbreviation $|ij\rangle = |i\rangle \otimes |j\rangle$ is quite common. The *m*-fold tensor product of a vector space is denoted by $V \otimes V \otimes \ldots \otimes V = V^{\otimes m}$.

E.g.
$$\begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \otimes \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \phi_1\psi_1 \\ \phi_1\psi_2 \\ \phi_2\psi_1 \\ \phi_2\psi_2 \end{pmatrix}$$

Separable

Some quantum states can be factored into (the tensor product of) individual qubit states. If we work on the states in reverse order by multiplying out the states and showing that you get the original state. Such factorizable states are called separable.

Entangled

A state is said to be entangled if it is not separable. There exist quantum states that cannot be factored into product states. These are called entangled states.

Week 4

Exercise 3.17. Is

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix}$$

a quantum gate? If so, what is $U|0\rangle$, and what is $U|1\rangle$?

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix}$$

$$U^{\dagger} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1^* & i^* \\ i^* & -1^* \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix}$$

$$U^{\dagger}U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix}$$

$$U^{\dagger}U = \frac{1}{2}\begin{pmatrix} 1-(-1) & i+i \\ -i-i & 1+1 \end{pmatrix}$$

$$U^{\dagger}U = \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} \neq I, \textit{ so it is not a quantum gate}$$

Exercise 3.18. Is

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$$

a quantum gate? If so, what is $U|0\rangle$, and what is $U|1\rangle$?

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$$

$$U^{\dagger} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1^* & i^* \\ 1^* & -i^* \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}$$

$$U^{\dagger}U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$$

$$U^{\dagger}U = \frac{1}{2}\begin{pmatrix} 1+1 & 1-1 \\ 1-1 & 1+1 \end{pmatrix}$$

$$U^{\dagger}U = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I, \textit{ so it is a quantum gate}$$

$$U|0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$U|0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$U|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$$

$$U|0\rangle = |i\rangle$$

$$U|1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$U|1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

$$U|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)$$

$$U|1\rangle = -|i\rangle$$

Exercise 4.3. Calculate the following inner products:
(a) $\langle 10|11\rangle$.
(b) $\langle +-|01\rangle$.
(c) $\langle 1+0|1-0\rangle$.

a) $\langle 10| = (0(1\ \ 0)\ 1(1\ \ 0)) = (0\ 0\ 1\ 0)$

$|11\rangle = \begin{pmatrix} 0\binom{0}{1} \\ 1\binom{0}{1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$

$\langle 10|11\rangle = 0$

b) $\langle +-| = (\frac{1}{\sqrt{2}}(\frac{1}{\sqrt{2}}\ \frac{-1}{\sqrt{2}})\frac{1}{\sqrt{2}}(\frac{1}{\sqrt{2}}\ \frac{-1}{\sqrt{2}}) = (\frac{1}{2}\ \frac{-1}{2}\ \frac{1}{2}\ \frac{-1}{2})$

$|01\rangle = \begin{pmatrix} 1\binom{0}{1} \\ 0\binom{0}{1} \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$

$\langle +-|01\rangle = \frac{-1}{2}$

c) $\langle 1+0| = (0\ 1)(\frac{1}{\sqrt{2}}(1\ 0)\frac{1}{\sqrt{2}}(1\ 0) = (0\ 1)(\frac{1}{\sqrt{2}}\ 0\ \frac{1}{\sqrt{2}}\ 0)$

$= 0(\frac{1}{\sqrt{2}}\ 0\ \frac{1}{\sqrt{2}}\ 0)1(\frac{1}{\sqrt{2}}\ 0\ \frac{1}{\sqrt{2}}\ 0)$

$= (0\ 0\ 0\ 0\ \frac{1}{\sqrt{2}}\ 0\ \frac{1}{\sqrt{2}}\ 0)$

$$|1-0\rangle = \binom{0}{1}\begin{pmatrix} \frac{1}{\sqrt{2}}\binom{0}{1} \\ \frac{-1}{\sqrt{2}}\binom{0}{1} \end{pmatrix} = \binom{0}{1}\begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ 0 \\ \frac{-1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \frac{1}{\sqrt{2}} \\ 0 \\ \frac{-1}{\sqrt{2}} \end{pmatrix}$$

$\langle 1+0|1-0\rangle = 0$

Exercise 4.12. Are each of the following states a product state or entangled state? If it is a product state, give the factorization.

(a) $\frac{1}{4}\left(3|00\rangle - \sqrt{3}|01\rangle + \sqrt{3}|10\rangle - |11\rangle\right)$.

(b) $\frac{1}{\sqrt{3}}|0\rangle|+\rangle + \sqrt{\frac{2}{3}}|1\rangle|-\rangle$.

a)

Two qubits are in the state $\frac{1}{4}(3|00\rangle - \sqrt{3}|01\rangle + \sqrt{3}|10\rangle - |11\rangle)$

Try to write this $|\psi_1\rangle|\psi_0\rangle$, where $|\psi_1\rangle = \alpha_1|0\rangle + \beta_1|1\rangle$,

$|\psi_0\rangle = \alpha_0|0\rangle + \beta_0|1\rangle$.

$$|\psi_1\rangle|\psi_0\rangle = (\alpha_1|0\rangle + \beta_1|1\rangle)(\alpha_0|0\rangle + \beta_0|1\rangle)$$
$$= \alpha_1\alpha_0|00\rangle + \alpha_1\beta_0|01\rangle + \beta_1\alpha_0|10\rangle + \beta_1\beta_0|11\rangle$$

$\alpha_1\alpha_0 = \frac{3}{4}$, $\alpha_1\beta_0 = \frac{-\sqrt{3}}{4}$, $\beta_1\alpha_0 = \frac{\sqrt{3}}{4}$, $\beta_1\beta_0 = \frac{-1}{4}$

For $\alpha_1\alpha_0 = \frac{3}{4}$, we have $\alpha_1 = \frac{3}{4\alpha_0}$ — ①

Sub ① into $\alpha_1\beta_0$, $\frac{3}{4\alpha_0}\beta_0 = \frac{-\sqrt{3}}{4}$

$\beta_0 = \frac{-\sqrt{3}}{3}\alpha_0$ — ②

~~Sub ② into $\beta_1\beta_0$, $2\beta_1\left(\frac{-\sqrt{3}}{3}\alpha_0\right) = 24$~~

~~$\beta_1 = \frac{3}{\sqrt{3}\alpha_0}$ — ③~~

For $\beta_1\alpha_0$, we have $\beta_1 = \frac{\sqrt{3}}{4\alpha_0}$ — ③

Sub ② and ③ into $\beta_1\beta_0$, $\left(\frac{\sqrt{3}}{4\alpha_0}\right)\left(\frac{-\sqrt{3}}{3}\alpha_0\right) = \frac{-1}{4}$, which is a true statement.

$|\psi_1\rangle|\psi_0\rangle = \left(\frac{3}{4\alpha_0}|0\rangle + \frac{\sqrt{3}}{4\alpha_0}|1\rangle\right)\left(\alpha_0|0\rangle - \frac{\sqrt{3}}{3}\alpha_0|1\rangle\right)$

Since α_0 cancels, yielding,

$|\psi_1\rangle|\psi_0\rangle = \left(\frac{3}{4}|0\rangle + \frac{\sqrt{3}}{4}|1\rangle\right)\left(|0\rangle - \frac{\sqrt{3}}{3}|1\rangle\right)$

Moving the factor of $\frac{\sqrt{3}}{2}$ to the right qubit so that both qubits are normalized,

$|\psi_1\rangle|\psi_0\rangle = \left(\frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle\right)\left(\frac{\sqrt{3}}{2}|0\rangle - \frac{1}{2}|1\rangle\right)$

$\therefore$ This is a product state.

b)

Two qubits are in the state $\frac{1}{\sqrt{3}}|0\rangle|+\rangle + \sqrt{\frac{2}{3}}|1\rangle|-\rangle$.

$$|0\rangle|+\rangle = 1\begin{pmatrix}\frac{1}{\sqrt2}\\ \frac{1}{\sqrt2}\end{pmatrix} \; 0\begin{pmatrix}\frac{1}{\sqrt2}\\ \frac{1}{\sqrt2}\end{pmatrix} = \begin{pmatrix}\frac{1}{\sqrt2}\\ \frac{1}{\sqrt2}\\ 0\\ 0\end{pmatrix}$$

$$|1\rangle|-\rangle = 0\begin{pmatrix}\frac{1}{\sqrt2}\\ \frac{-1}{\sqrt2}\end{pmatrix} \; 1\begin{pmatrix}\frac{1}{\sqrt2}\\ \frac{-1}{\sqrt2}\end{pmatrix} = \begin{pmatrix}0\\ 0\\ \frac{1}{\sqrt2}\\ \frac{-1}{\sqrt2}\end{pmatrix}$$

$$\frac{1}{\sqrt3}|0\rangle|+\rangle + \sqrt{\frac{2}{3}}|1\rangle|-\rangle = \begin{pmatrix}\frac{1}{\sqrt6}\\ \frac{1}{\sqrt6}\\ \sqrt{\frac{2}{6}}\\ -\sqrt{\frac{2}{6}}\end{pmatrix}$$

Try to write $|\psi_1\rangle|\psi_0\rangle = (\alpha_1|0\rangle + \beta_1|1\rangle)(\alpha_0|0\rangle + \beta_0|1\rangle)$

$$= \alpha_1\alpha_0|00\rangle + \alpha_1\beta_0|01\rangle + \beta_1\alpha_0|10\rangle + \beta_1\beta_0|11\rangle$$

$\alpha_1\alpha_0 = \frac{1}{\sqrt6}$, $\alpha_1\beta_0 = \frac{1}{\sqrt6}$, $\beta_1\alpha_0 = \sqrt{\frac{2}{6}}$, $\beta_1\beta_0 = -\sqrt{\frac{2}{6}}$.

For $\alpha_1\alpha_0 = \frac{1}{\sqrt6}$, we have $\alpha_1 = \frac{1}{\sqrt6\,\alpha_0}$ —①

Sub ① into $\alpha_1\beta_0$, $\frac{1}{\sqrt6\,\alpha_0}\cdot\beta_0 = \frac{1}{\sqrt6}$

$\beta_0 = \alpha_0$ —②

~~Sub ②~~ For $\beta_1\alpha_0 = \sqrt{\frac{2}{6}}$, $\beta_1 = \sqrt{\frac{2}{6}}\cdot\frac{1}{\alpha_0}$ —③

Sub ② and ③ into $\beta_1\beta_0$, $\sqrt{\frac{2}{6}}\cdot\frac{1}{\alpha_0}\cdot\alpha_0$

$= \sqrt{\frac{2}{6}} \neq -\sqrt{\frac{2}{6}}$, which is false.

$\because$ This cannot be written in product state that ~~property~~ state of the qubits are intermined.

$\therefore$ This is an entangled state.

$$CNOT\,(X\otimes I) = CNOT\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1&0\\0&1\end{pmatrix} = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}\begin{pmatrix}0&0&1&0\\0&0&0&1\\1&0&0&0\\0&1&0&0\end{pmatrix} = \begin{pmatrix}0&0&1&0\\0&0&0&1\\0&1&0&0\\1&0&0&0\end{pmatrix}$$

$$(X\otimes X)\,CNOT = \begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}CNOT = \begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix} = \begin{pmatrix}0&0&1&0\\0&0&0&1\\0&1&0&0\\1&0&0&0\end{pmatrix}$$

$\therefore CNOT\,(X\otimes I) = (X\otimes X)\,CNOT$

Exercise 4.8. Normalize the following quantum state:

$$A\left(\frac{1}{2}|00\rangle + i|01\rangle + \sqrt{2}|10\rangle - |11\rangle\right).$$

$$|A|^2 * \frac{1}{2}^2 + |A|^2 * i^2 + |A|^2 * \sqrt{2}^2 + |A|^2 * (-1)^2 = 1$$

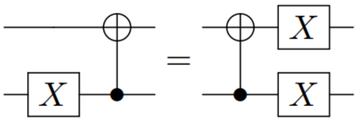
$$|A|^2\left(\frac{1}{4} + 1 + 2 + 1\right) = 1$$

$$|A|^2 = \frac{4}{17}$$

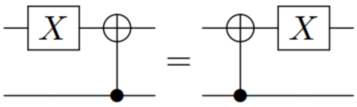
$$A = \frac{2}{\sqrt{17}}$$

Exercise 4.15. Prove the following circuit identities, such as by finding the matrix representation of each circuit.

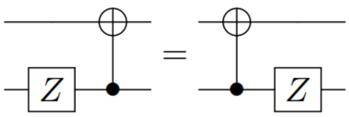
(a) $\text{CNOT}(X \otimes I) = (X \otimes X)\text{CNOT}$.



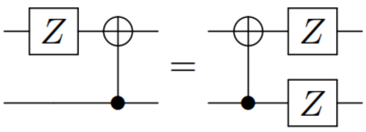
(b) $\text{CNOT}(I \otimes X) = (I \otimes X)\text{CNOT}$.



(c) $\text{CNOT}(Z \otimes I) = (Z \otimes I)\text{CNOT}$.



(d) $\text{CNOT}(I \otimes Z) = (Z \otimes Z)\text{CNOT}$.



a) $\text{CNOT}(X \otimes I) = \text{CNOT}\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1&0\\0&1\end{pmatrix} = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}\begin{pmatrix}0&0&1&0\\0&0&0&1\\1&0&0&0\\0&1&0&0\end{pmatrix} = \begin{pmatrix}0&0&1&0\\0&0&0&1\\0&1&0&0\\1&0&0&0\end{pmatrix}$

$(X \otimes X)\text{CNOT} = \begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}\text{CNOT} = \begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix} = \begin{pmatrix}0&0&1&0\\0&0&0&1\\0&1&0&0\\1&0&0&0\end{pmatrix}$

$\therefore \text{CNOT}(X \otimes I) = (X \otimes X)\text{CNOT}$

b) $\mathrm{CNOT}(I\otimes X) = \mathrm{CNOT}\begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix} = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix} = \begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}$

$(I\otimes X)\,\mathrm{CNOT} = \begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix} = \begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}$

$\therefore \mathrm{CNOT}(I\otimes X) = (I\otimes X)\,\mathrm{CNOT}$.

c) $\mathrm{CNOT}(Z\otimes I) = \mathrm{CNOT}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}1&0\\0&1\end{pmatrix} = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix} = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&-1\\0&0&-1&0\end{pmatrix}$

$(Z\otimes I)\,\mathrm{CNOT} = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix} = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&-1\\0&0&-1&0\end{pmatrix}$

$\therefore \mathrm{CNOT}(Z\otimes I) = (Z\otimes I)\,\mathrm{CNOT}$.

d) $\mathrm{CNOT}(I\otimes Z) = \mathrm{CNOT}\begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix} = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&1&0\\0&0&0&-1\end{pmatrix} = \begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&0&-1\\0&0&1&0\end{pmatrix}$

$(Z\otimes Z)\,\mathrm{CNOT} = \begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\mathrm{CNOT} = \begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix} = \begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&0&-1\\0&0&1&0\end{pmatrix}$

$\therefore \mathrm{CNOT}(I\otimes Z) = (Z\otimes Z)\,\mathrm{CNOT}$.

Exercise 4.20. What is the controlled-Z gate as a matrix?

Ex 4.20

$CZ|00\rangle = |00\rangle$

$CZ|01\rangle = |01\rangle$

$CZ|10\rangle = |1\rangle \otimes Z|0\rangle$

$CZ|11\rangle = |1\rangle \otimes Z|1\rangle$.

~~Z work as a single qubit as~~
~~$Z|0\rangle = a|0\rangle$~~

To get matrix represatation of CZ, first say Z acts on a single qubit as

$Z|0\rangle = a|0\rangle + b|1\rangle$,

$Z|1\rangle = c|0\rangle + d|1\rangle$.

Z as 2×2 matrix is $Z = \begin{pmatrix}a&c\\b&d\end{pmatrix}$

$CZ|10\rangle = |1\rangle\otimes(a|0\rangle + b|1\rangle) = a|10\rangle + b|11\rangle$.

$CZ|11\rangle = |1\rangle\otimes(c|0\rangle + d|1\rangle) = c|10\rangle + d|11\rangle$

$$CZ = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&a&b\\0&0&c&d\end{pmatrix}$$

$$= \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&-1\end{pmatrix}$$

Exercise 4.22. The Mølmer-Sørensen (MS) gate is a two-qubit gate that can be naturally implemented on trapped ion quantum computers. It transforms Z-basis states by

$$|00\rangle \to \frac{1}{\sqrt{2}}(|00\rangle + i|11\rangle),$$
$$|01\rangle \to \frac{1}{\sqrt{2}}(|01\rangle - i|10\rangle),$$
$$|10\rangle \to \frac{1}{\sqrt{2}}(|10\rangle - i|01\rangle),$$
$$|11\rangle \to \frac{1}{\sqrt{2}}(|11\rangle + i|00\rangle).$$

What is the MS gate as a matrix?

Ex 4.22

$$MS\,(c_0|00\rangle + c_1|01\rangle + c_2|10\rangle + c_3|11\rangle)$$
$$= c_0 MS|00\rangle + c_1 MS|01\rangle + c_2 MS|10\rangle + c_3 MS|11\rangle$$
$$= c_0 \frac{1}{\sqrt{2}}(|00\rangle + i|11\rangle) + c_1 \frac{1}{\sqrt{2}}(|01\rangle - i|10\rangle) + c_2 \frac{1}{\sqrt{2}}(|10\rangle - i|01\rangle) + c_3 \frac{1}{\sqrt{2}}(|11\rangle + i|00\rangle)$$
$$= \frac{1}{\sqrt{2}}\left((c_0 + ic_3)|00\rangle + (c_1 - ic_2)|01\rangle + (-ic_1 + c_2)|10\rangle + (ic_0 + c_3)|11\rangle\right)$$

$$= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 & i \\ 0 & 1 & -i & 0 \\ 0 & -i & 1 & 0 \\ i & 0 & 0 & 1 \end{pmatrix}.$$

Exercise 4.25. Say there is a unitary U that is able to clone qubits in two known states $|\psi\rangle$ and $|\phi\rangle$. That is,

$$U|\psi\rangle|0\rangle = |\psi\rangle|\psi\rangle,$$
$$U|\phi\rangle|0\rangle = |\phi\rangle|\phi\rangle.$$

For example, an operator that can clone both $|0\rangle$ and $|1\rangle$ is CNOT, since CNOT$|00\rangle = |00\rangle$ and CNOT$|10\rangle = |11\rangle$. Taking the inner product of the previous two equations,

$$\langle\psi|\langle 0|U^\dagger U|\phi\rangle|0\rangle = (\langle\psi|\langle\psi|)(|\phi\rangle|\phi\rangle)$$
$$(\langle\psi|\langle 0|)(|\phi\rangle|0\rangle) = (\langle\psi|\langle\psi|)(|\phi\rangle|\phi\rangle)$$
$$\langle\psi|\phi\rangle\langle 0|0\rangle = \langle\psi|\phi\rangle\langle\psi|\phi\rangle$$
$$\langle\psi|\phi\rangle = (\langle\psi|\phi\rangle)^2.$$

For $\langle\psi|\phi\rangle$ to be equal to its square, it must equal 0 or 1. Thus, $|\psi\rangle = |\phi\rangle$, or $|\psi\rangle$ and $|\phi\rangle$ are orthogonal. Thus, an operator can only clone states that are orthogonal.

Does there exist a quantum operator U that can clone both

(a) $|+\rangle$ and $|-\rangle$?
(b) $|i\rangle$ and $|-i\rangle$?
(c) $|0\rangle$ and $|+\rangle$?

---

a) $\langle +|-\rangle = (\frac{1}{\sqrt{2}} \;\; \frac{1}{\sqrt{2}})\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix} = 0$

Thus, $|+\rangle$ and $|-\rangle$ are orthogonal.
Ans: Yes

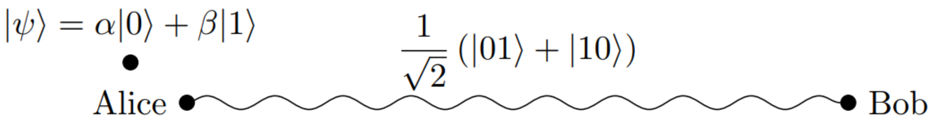
b) $\langle i|-i\rangle = (\frac{1}{\sqrt{2}} \;\; \frac{i}{\sqrt{2}})\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \end{pmatrix} = (\frac{1}{2} - \frac{i^2}{2}) = 1$

Thus, $|i\rangle$ and $|-i\rangle$ are orthogonal.
Ans: Yes

c) $\langle 0|+\rangle = (1 \;\; 0)\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}$

Thus, $|i\rangle$ and $|-i\rangle$ are not orthogonal.
Ans: No

Exercise 6.16. Alice wants to teleport a qubit in an unknown state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ to Bob. Instead of sharing two entangled qubits in the $|\Phi^+\rangle$ state, they share two entangled qubits in the $|\Psi^+\rangle$ state:



Altogether, the initial state of the system is

$$\begin{aligned}|\psi\rangle|\Psi^+\rangle &= (\alpha|0\rangle + \beta|1\rangle)\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \\ &= \frac{1}{\sqrt{2}}(\alpha|001\rangle + \alpha|010\rangle + \beta|101\rangle + \beta|110\rangle).\end{aligned}$$

So, the left two qubits are Alice's, and the right qubit is Bob's.

(a) Show that if Alice applies CNOT to her two qubits, followed by H to her left qubit, the state of the system becomes

$$\frac{1}{2}\big[|00\rangle(\beta|0\rangle + \alpha|1\rangle) + |01\rangle(\alpha|0\rangle + \beta|1\rangle) \\ + |10\rangle(-\beta|0\rangle + \alpha|1\rangle) + |11\rangle(\alpha|0\rangle - \beta|1\rangle)\big].$$

(b) Next, Alice measures both of her qubits. What values can she get, with what probabilities, and what does the state collapse to in each case?

(c) Finally, Alice tells Bob the results of her measurement. For each possible result, what should Bob do to his qubit so that is $\alpha|0\rangle + \beta|1\rangle$, the state that Alice wanted to teleport to him?

---

a) Apply CNOT to Alice's two qubits, of the following state of system

$$\frac{1}{\sqrt{2}}(\alpha|001\rangle + \alpha|010\rangle + \beta|101\rangle + \beta|110\rangle)$$

$$= \frac{1}{\sqrt{2}}(\alpha|001\rangle + \alpha|010\rangle + \beta|111\rangle + \beta|100\rangle$$

Now, apply H to leftmost qubit,

$$\frac{1}{\sqrt{2}}\left(\alpha \frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)|01\rangle + \alpha\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)|10\rangle + \beta\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)|11\rangle + \beta\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)|00\rangle\right)$$

$$= \frac{1}{2}(\alpha|001\rangle + \alpha|101\rangle + \alpha|010\rangle + \alpha|110\rangle + \beta|011\rangle - \beta|111\rangle + \beta|000\rangle - \beta|100\rangle)$$

$$= \frac{1}{2}(\beta|000\rangle + \alpha|001\rangle + \alpha|010\rangle + \beta|011\rangle - \beta|100\rangle + \alpha|101\rangle + \alpha|110\rangle - \beta|111\rangle)$$

$$= \frac{1}{2}\left[|00\rangle(\beta|0\rangle+\alpha|1\rangle) + |01\rangle(\alpha|0\rangle+\beta|1\rangle) + |10\rangle(-\beta|0\rangle+\alpha|1\rangle) + |11\rangle(\alpha|0\rangle-\beta|1\rangle)\right]$$

b) Coefficient is $\frac{1}{2}$, $|\frac{1}{2}|^2 = \frac{1}{4}$.

She can get $|00\rangle$ with probability $\frac{1}{4}$, collapse to $|00\rangle(\beta|0\rangle+\alpha|1\rangle)$

$|01\rangle$ with probability $\frac{1}{4}$, collapse to $|01\rangle(\alpha|0\rangle+\beta|1\rangle)$

$|10\rangle$ with probability $\frac{1}{4}$, collapse to $|10\rangle(-\beta|0\rangle+\alpha|1\rangle)$

$|11\rangle$ with probability $\frac{1}{4}$, collapse to $|11\rangle(\alpha|0\rangle-\beta|1\rangle)$.

c) For $|00\rangle(\beta|0\rangle+\alpha|1\rangle)$, apply X gate so that, $= |00\rangle(\alpha|0\rangle+\beta|1\rangle)$.

For $|01\rangle(\alpha|0\rangle+\beta|1\rangle)$, apply nothing.

For $|10\rangle(-\beta|0\rangle+\alpha|1\rangle)$, apply X gate so that, $= |10\rangle(\alpha|0\rangle-\beta|1\rangle)$

and then apply Z gate so that, $= |10\rangle(\alpha|0\rangle+\beta|1\rangle)$.

For $|11\rangle(\alpha|0\rangle-\beta|1\rangle)$, apply Z gate so that, $= |11\rangle(\alpha|0\rangle+\beta|1\rangle)$.

P.S. All the above gate applied to Bob's qubit only.

Week 5

Exercise 6.25. You are Alice, and you and Bob are establishing a secret key using BB84. You have the following random bits and random bases. What qubits do you send to Bob?

Alice's Bits	1	0	0	1	0	0	0	1	1
Alice's Bases	X	X	Z	Z	Z	X	X	X	X
Alice Sends	?	?	?	?	?	?	?	?	?

Alice Sends: |-> |+> |0> |1> |0> |+> |+> |-> |->

Exercise 6.26. You are Bob, and you and Alice are establishing a secret key using BB84. You choose the following random bases to measure each qubit in, and you got the following results.

Bob's Bases	X	X	Z	X	Z	Z	X	X	Z
Bob's Measurement	$\|+\rangle$	$\|-\rangle$	$\|0\rangle$	$\|-\rangle$	$\|0\rangle$	$\|1\rangle$	$\|1\rangle$	$\|+\rangle$	$\|1\rangle$
Bob's Bits	0	1	0	1	0	1	1	0	1

Next, you call Alice and learn that she used the following bases:

Alice's Bases	Z	Z	Z	Z	Z	X	X	Z	Z

What is your shared secret key?

Shared secret key: 0011

Exercise 7.3. Quantum oracles are quantum gates, so they act across superpositions. Consider an input qubit in the superposition state

$$\frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle,$$

and an answer qubit in the state $|-\rangle$. Show that the quantum oracle acts by

$$\left(\frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle\right)|-\rangle \xrightarrow{U_f} \left(\frac{\sqrt{3}}{2}(-1)^{f(0)}|0\rangle + \frac{1}{2}(-1)^{f(1)}|1\rangle\right)|-\rangle.$$

$$\left(\frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle\right)|-\rangle = \left(\frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle\right)\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

$$= \frac{\sqrt{3}}{2\sqrt{2}}(|0\rangle|0\rangle - |0\rangle|1\rangle) + \frac{1}{2\sqrt{2}}(|1\rangle|0\rangle - |1\rangle|1\rangle)$$

$$\xrightarrow{U_f} \frac{\sqrt{3}}{2\sqrt{2}}(|0\rangle|0\oplus f(0)\rangle - |0\rangle|1\oplus f(0)\rangle) + \frac{1}{2\sqrt{2}}(|1\rangle|0\oplus f(1)\rangle - |1\rangle|1\oplus f(1)\rangle)$$

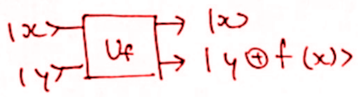
$$= \frac{\sqrt{3}}{2}|0\rangle\frac{1}{\sqrt{2}}(|0\oplus f(0)\rangle - |1\oplus f(0)\rangle) + \frac{1}{2}|1\rangle\frac{1}{\sqrt{2}}(|0\oplus f(1)\rangle - |1\oplus f(1)\rangle)$$

$$= \frac{\sqrt{3}}{2}(-1)^{f(0)}|0\rangle|-\rangle + \frac{1}{2}(-1)^{f(1)}|1\rangle|-\rangle$$

$$= \left[\frac{\sqrt{3}}{2}(-1)^{f(0)}|0\rangle + \frac{1}{2}(-1)^{f(1)}|1\rangle\right]|-\rangle.$$

Exercise 7.4. We saw that when the answer qubit is in the state $|-\rangle$, we get phase kickback. Let us explore what happens if the answer qubit is in the state $|+\rangle$. Suppose an input qubit and answer qubit are in the state $|x\rangle|+\rangle$, where x is a bit. If we apply the quantum oracle U_f to this, which maps $|x\rangle|y\rangle$ to $|x\rangle|y\oplus f(x)\rangle$, what do we get if

(a) $f(x) = 0$?
(b) $f(x) = 1$?
(c) How do your answers in parts (a) and (b) compare to the initial state $|x\rangle|+\rangle$?



Now, we consider $|x\rangle|+\rangle$ as input qubit and answer qubit

$$|x\rangle|+\rangle \xrightarrow{U_f} |x\rangle|+\oplus f(x)\rangle$$

$$= \begin{cases} |x\rangle|+\oplus 0\rangle, \text{ if } f(x)=0 \\ |x\rangle|+\oplus 1\rangle, \text{ if } f(x)=1 \end{cases}$$

$$= \begin{cases} |x\rangle\frac{1}{\sqrt{2}}(|0\oplus 0\rangle + |1\oplus 0\rangle) \\ |x\rangle\frac{1}{\sqrt{2}}(|0\oplus 1\rangle + |1\oplus 1\rangle) \end{cases}$$

$$= \begin{cases} |x\rangle\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ |x\rangle\frac{1}{\sqrt{2}}(|1\rangle + |0\rangle) \end{cases}$$

$$= \begin{cases} |x\rangle|+\rangle \\ |x\rangle|+\rangle \end{cases}$$

Question (a) if $f(x)=0$, we get $|x\rangle|+\rangle$
Question (b) if $f(x)=1$, we get $|x\rangle|+\rangle$

Exercise 7.7. Say you are trying to use Deutsch's algorithm, but you neglect the last Hadamard gate. That is, you apply

$$|0\rangle \xrightarrow{H} |+\rangle \xrightarrow{U_f} \frac{1}{\sqrt{2}}\left[(-1)^{f(0)}|0\rangle + (-1)^{f(1)}|1\rangle\right].$$

If you measure the system now, what possible states do you get, and with what probabilities?

First, we substitute $f(0) = b_0$ and $f(1) = b_1$:

$$\frac{1}{\sqrt{2}}\left[(-1)^{b_0}|0\rangle + (-1)^{b_1}|1\rangle\right]$$

$$= \frac{1}{\sqrt{2}}(-1)^{b_0}\left[|0\rangle + (-1)^{b_1-b_0}|1\rangle\right]$$

$$= \begin{cases} \frac{1}{\sqrt{2}}(-1)^{b_0}(|0\rangle + |1\rangle) \text{ if } b_0 = b_1 \\ \frac{1}{\sqrt{2}}(-1)^{b_0}(|0\rangle - |1\rangle) \text{ if } b_0 \neq b_1 \end{cases}$$

$$= \begin{cases} (-1)^{b_0}|+\rangle, \; b_0 = b_1 \\ (-1)^{b_0}|-\rangle, \; b_0 \neq b_1 \end{cases}$$

If we measure this, we get $|0\rangle$ with probability of $\frac{1}{2}$.
$|1\rangle$ with probability of $\frac{1}{2}$

Exercise 7.11. Apply $H \otimes H \otimes H$ to $|000\rangle$, and show that the resulting state is a uniform superposition of all binary strings of length 3. If you measure the qubits, what possible outcomes can you get, and with what probabilities?

Apply $H \otimes H \otimes H$ to $|000\rangle$:

$$H^{\otimes 3}|000\rangle = H|0\rangle H|0\rangle H|0\rangle$$
$$= |+\rangle|+\rangle|+\rangle$$
$$= |+++\rangle$$
$$= \frac{1}{\sqrt{2^3}}\left(|000\rangle + |001\rangle + |010\rangle + \dots + |111\rangle\right)$$
$$= \frac{1}{\sqrt{8}}\left(|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle + |111\rangle\right)$$

$\therefore$ Ans: Get one of the basis states $|000\rangle, |001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle, |111\rangle$ with each probability $\frac{1}{8}$.

Exercise 7.23. Answer the following questions about Grover's algorithm:

(a) When the n qubits are in their initial state (all $|+\rangle$ states), if you measure the qubits, what is the probability that you get $|w\rangle$? Express your answer in terms of $N = 2^n$.

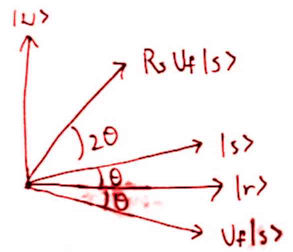
(b) Say you apply just one step of Grover's algorithm (one query U_f and one reflection R_s). If you measure the qubits after this one step, what is the probability that you get $|w\rangle$? Express your answer in terms of $N = 2^n$. Hint: In the rw-plane, the amplitude of the state in $|w\rangle$ is the sine of the angle between the state and $|r\rangle$.

a) $|s\rangle = |+\rangle^{\otimes n} = \frac{1}{\sqrt{N}} \sum_{x \in \{0,1\}} |x\rangle$, where $N = 2^n$

$$= \frac{1}{\sqrt{N}}\left(|w\rangle + \sum_{i \neq w} |i\rangle\right)$$
$$= \frac{1}{\sqrt{N}}|w\rangle + \frac{1}{\sqrt{N}}\sum_{i \neq w}|i\rangle$$
$$= \frac{1}{\sqrt{N}}|w\rangle \sqrt{\frac{N-1}{N}} \underbrace{\frac{1}{\sqrt{N-1}} \sum_{i \neq w}|i\rangle}_{|r\rangle}$$
$$= \frac{1}{\sqrt{N}}|w\rangle + \sqrt{\frac{N-1}{N}}|r\rangle$$

$\therefore$ Probability that I get $|w\rangle$ is $\left(\frac{1}{\sqrt{N}}\right)^2 = \frac{1}{N}$.

b)



$\sin\theta = \frac{1}{\sqrt{N}}$

Now, we find $\sin(3\theta)$, $= 3\sin\theta - 4\sin^3\theta$

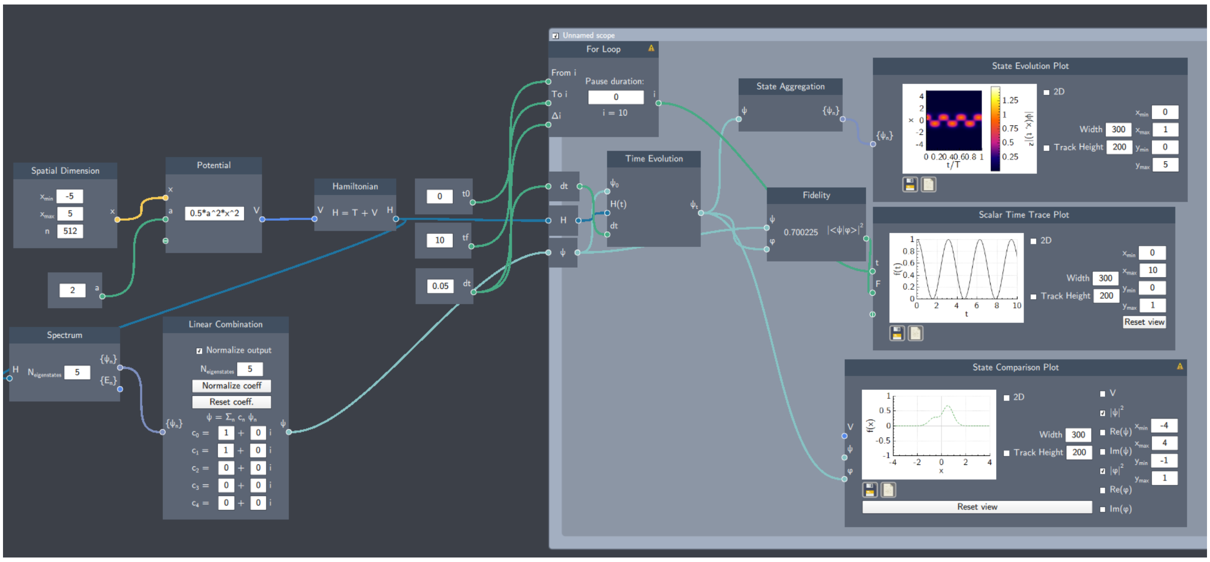
$$= 3\left(\frac{1}{\sqrt{N}}\right) - 4\left(\frac{1}{\sqrt{N}}\right)^3$$

$\therefore$ Probability of $|w\rangle$ after U_f and R_s

$$= \left|\frac{3}{\sqrt{N}} - \frac{4}{N^{\frac{3}{2}}}\right|^2$$
$$= \frac{9}{N} - \frac{24}{N^{\frac{1}{2}+\frac{3}{2}}} + \frac{16}{N^{\frac{6}{2}}}$$
$$= \frac{9}{N} - \frac{24}{N^2} + \frac{16}{N^3}$$

Week 7

1. Go to https://www.quatomic.com/composer/tutorial/ and watch the video. Try to install Composer on your desktop (it can be downloaded from Blackboard) and work through the tutorial yourself. Don't worry if you can't install Composer—we'll use the computers in the lecture room instead!



2. In two sentences, describe why quantum mechanics is necessary to explain matter (like atoms). Do some research: how small are electrons, protons, and atoms? What does this tell you about the quantum world?

Due to the inability of the classical physics concepts "particle" or "wave" to fully describe the behaviour of quantum-scale objects. Concepts such as wave-particle duality in quantum mechanics are necessary to explain matter (like atoms) may be partly described in terms of both particles and waves.

3. Go to https://phet.colorado.edu/sims/html/wave-on-a-string/latest/wave-on-a-string_all.html. What is the difference between what happens when you pulse a wave with a fixed end vs. a loose end?

Pulse a wave with a fixed end → wave reflects back inverted.
Pulse a wave with a loose end → wave reflects back without inverting its phase.

4. A wave traveling to the left has the form $f(x,t) = A\cos(kx + \omega t)$ and a wave travelling to the right has the form $g(x,t) = A\cos(kx - \omega t)$. Using trigonometric identities (see https://en.wikipedia.org/wiki/List_of_trigonometric_identities), show that when you add these waves, you get a standing wave of the form $h(x,t) = a\cos(bx)\cos(ct)$. What are the values of a, b and c? What does this tell you about the amplitude and wavelength of the standing wave relative to the amplitude wavelength of the travelling waves that make it up?

A wave travelling to left: $f(x,t) = A\,cos(kx + \omega t)$
A wave travelling to right: $g(x,t) = A\,cos(kx - \omega t)$

To add these waves using trigonometric identities,

$$\cos\theta + \cos\varphi = 2\cos\left(\frac{\theta+\varphi}{2}\right)\cos\left(\frac{\theta-\varphi}{2}\right)$$

$h(x,t) = f(x,t) + g(x,t)$
$h(x,t) = 2A\,cos(\frac{kx+\omega t+kx-\omega t}{2})cos(\frac{kx+\omega t-kx+\omega t}{2})$
$h(x,t) = 2A\,cos(kx)cos(\omega t)$

To answer the question, the values of a = 2A; b = k; c = ω.

Value of a tells me that the maximum amplitude of the standing wave is twice the amplitude of the individual travelling wave.

Value of b tells me the wavenumber remains unchanged.

Value of c tells me the angular frequency remains unchanged.

Wavelength of the standing wave $\lambda = \frac{2\pi}{k}$, just the same.

5. Using dimensional analysis, find the speed v of a wave on a string with length l, mass m, and tension Q. Find the frequency of the fundamental and first excited modes of the string (use dimensional analysis again—how do you relate wave speed and the other parameters given to frequency? We do this because dimensional analysis is a great way to check if you're doing the right thing, both classically and in quantum mechanics.

Using dimensional analysis with SI unit,

$v = f\lambda = ms^{-1} = length * time^{-1}$

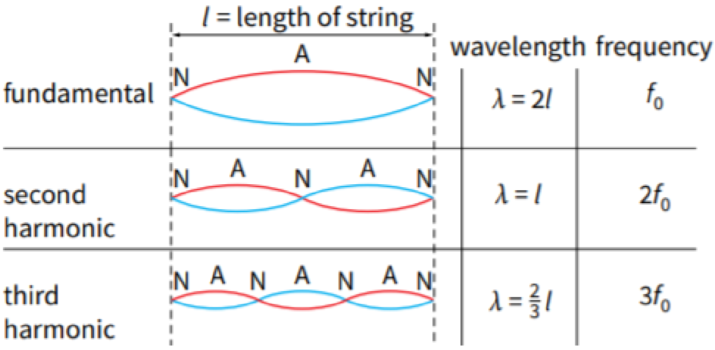
Tension is a type of contact force, $Q = F_T = ma = kg\, ms^{-2} = mass * length * time^{-2}$

$\mu = \frac{m}{l} = kg\, m^{-1} = mass * length^{-1}$

$\sqrt{\frac{Q}{\mu}} = \sqrt{\frac{mass*length*time^{-2}}{mass*length^{-1}}} = \sqrt{length^2 * time^{-2}} = length * time^{-1} = v$

$\therefore v = \sqrt{\frac{Q}{\mu}} = \sqrt{\frac{Q}{m*l^{-1}}}$

Now, to find the frequency of the fundamental and first excited mode (2nd Harmonic) of the string.



For the fundamental mode of string,

$f^2 = \frac{v^2}{\lambda^2} = \frac{v^2}{(2l)^2} = \frac{Q}{4m*l}$

$f = \sqrt{\frac{Q}{4m*l}}$

For the first excited mode of string,

$f^2 = \frac{v^2}{\lambda^2} = \frac{v^2}{l^2} = \frac{Q}{m*l}$

$f = \sqrt{\frac{Q}{m*l}}$

6. Using the results you got from 5, estimate the speed of a wave on a guitar string. Determine the length l required to hit an A4 note (440 Hz). Assume a tension of 150 N and a linear density of 7.20 g/m of the string. How does this change if you try to hit an A3 note (220 Hz)? What about an A5 note (880 Hz)? How do guitars allow you to hit various notes without making enormously long guitars?

Speed of wave on guitar string for a string pinned at 2 ends.

Linear density (μ) SI unit is kg m^-1, 7.20 g m^-1 = 0.00720 kg m^-1

$$v = \sqrt{\frac{Q}{\mu}}$$

$$v = \sqrt{\frac{150}{0.00720}}$$

$$v = 144.338ms^{-1}$$

In order to hit an A4 note, consider the fundamental mode of the string.

$$f = \frac{v}{2l}$$

$$l = \frac{144.338}{2*440} = 0.164m$$

For hitting an A3 note

$$l = \frac{144.338}{2*220} = 0.328m$$

For hitting an A5 note

$$l = \frac{144.338}{2*880} = 0.082m$$

When playing a longer string on guitar, it vibrates slowly, creating pressure waves that are farther apart, so that it has a low frequency. On the other hand, when playing a short string on guitar, it vibrates faster, creating pressure waves that are closer together, and hence it has a higher frequency. The pitch of sound is determined by the frequency of vibration of the sound waves that produce them. This is how guitars allow us to hit various notes without making enormously long guitars.

7. Define, in your own words, the following terms:

- Harmonic
- standing wave
- travelling wave
- quantum
- normalization
- wavefunction

Harmonic:

A harmonic is a wave that has multiples of a fundamental frequency that a vibrating object produces. The n^{th} harmonic has a frequency $f_n = n * f_1$ where f_1 is the fundamental frequency.

Standing wave:

A standing wave is the combination of two waves that are moving in opposite directions. The peaks and troughs of the standing wave oscillate around the same point.

Travelling wave:

A travelling wave is a wave moving. The peaks and troughs of the travelling wave move through a medium at a constant speed, when it meets a boundary the wave will be reflected.

Quantum:

The smallest discrete unit of a phenomenon.

Normalisation:

Normalisation refers to the mathematical step made to ensure that all probabilities sum to 1.

Wavefunction:

A mathematical model of a particular wave is called a "wave function". The symbol "function" is denoted by f. In most cases, an equation is used to express it. It can be a function of time (t), distance (d), etc. The function is a wave function if the equation describes a wave.

8. We'll be doing some calculus starting next week, so the following exercises are meant to warm you up a bit for this. Solve the following:

(a) $\int x\,dx$

(b) $\int_0^2 x\,dx$ (what's the difference between (a) and (b)?

(c) $\frac{d}{dx}[A\sin(ax) + B\cos(bx)]$

(d) $\frac{d^2}{dx^2}[A\sin(ax) + B\cos(bx)]$

(e) Show that for an equation of the form $\frac{d^2 f}{dx^2} = -Af$, solutions should take the form $f(x) = a_1\sin(a_2 x) + b_1\cos(b_2 x)$. If $f(0) = f(L) = 0$, and we enforce that $\int_{-\infty}^{\infty} f(x)\,dx = 1$, what should a_1, a_2, b_1, and b_2 be? Do you need to specify all of these variables?

(f) What is $\frac{d}{dx}e^x$? What about $\frac{d}{dx}e^{Ax}$? How about $\frac{d}{dx}e^{f(x)}$, where $f(x)$ is just some function of x? Here e is Euler's number $e = 2.71828$.

(g) What is $\frac{d}{dx}\ln(x)$? How about $\frac{d}{dx}\ln(f(x))$? Here, $\ln(\cdot)$ means the natural log.

a. $\int xdx = \frac{x^2}{2} + C$

b. $\int_0^2 xdx = [\frac{x^2}{2}]_0^2 = \frac{2^2}{2} - \frac{0^2}{2} = 2$

(a) is an indefinite integral. No bounds.
(b) is a definite integral. Bounded from 0 to 2.

c. $\frac{d}{dx}[A\,sin(ax) + B\,cos(bx)]$

$= A\frac{d}{dx}[sin(ax)] + B\frac{d}{dx}[cos(bx)]$

$= A\,cos(ax)\frac{d}{dx}(ax) + B[-\,sin(bx)]\frac{d}{dx}(bx)$

$= A\,a\,cos(ax) - B\,b\,sin(bx)$

d. $\frac{d^2}{dx^2}[A\,sin(ax) + B\,cos(bx)]$

$= \frac{d}{dx}[A\,a\,cos(ax) - B\,b\,sin(bx)]$

$= A\,a[-\,sin(ax)]\frac{d}{dx}(ax) - B\,b\,cos(bx)\frac{d}{dx}(bx)$

$=- A\,a^2 sin(ax) - B\,b^2 cos(bx)$

e. $f(x) = a_1 sin(a_2 x) + b_1 cos(b_2 x)$

$f'(x) = a_1 a_2 cos(a_2 x) - b_1 b_2 sin(b_2 x)$

$f''(x) =- a_1 a_2^2 sin(a_2 x) - b_1 b_2^2 cos(b_2 x)$

$\because Given\ f''(x) =- Af$

$\therefore\ - a_1 a_2^2 sin(a_2 x) - b_1 b_2^2 cos(b_2 x) =- A[a_1 sin(a_2 x) + b_1 cos(b_2 x)]$

For sin,

$- a_1 a_2^2 =- A\ a_1$

$a_2^2 = A$

$a_2 =\pm \sqrt{A}$

For cos,

$- b_1 b_2^2 =- Ab_1$

$b_2^2 = A$

$b_2 =\pm \sqrt{A}$

a_1 and b_1 are cancelled out in the equivalent equations above. So, we do not need to specify all of these variables.

f. $\frac{d}{dx} e^x = e^x$

$\frac{d}{dx} e^{Ax} = Ae^{Ax}$

$\frac{d}{dx} e^{f(x)} = e^{f(x)} \frac{d}{dx} f(x) = e^{f(x)} f'(x)$

g. $\frac{d}{dx} ln(x) = \frac{1}{x}$

$\frac{d}{dx} ln(f(x)) = \frac{1}{f(x)} \frac{d}{dx} f(x) = \frac{f'(x)}{f(x)}$

9. Show that a function of the form $f(x) = Ae^{-Bx^2}$ satisfies the equation $-a\frac{d^2f}{dx^2} + bx^2 f = cf$. What are A and B in terms of a, b, and c, if we again enforce that $\int_{-\infty}^{\infty} f(x)\,dx = 1$?

$f(x) = Ae^{-Bx^2}$

$f'(x) = Ae^{-Bx^2}\frac{d}{dx}(-Bx^2) =- 2ABxe^{-Bx^2}$

$f''(x) =- 2AB\frac{d}{dx}(xe^{-Bx^2}) =- 2AB(e^{-Bx^2}\frac{d}{dx}x + x\frac{d}{dx}e^{-Bx^2}) =- 2AB(e^{-Bx^2} + xe^{-Bx^2}\frac{d}{dx}(-Bx^2))$

$=- 2AB(e^{-Bx^2} - 2Bx^2e^{-Bx^2})$

$-a\frac{d^2f}{dx^2} + bx^2f$

$= (-a)[-2AB(e^{-Bx^2} - 2Bx^2e^{-Bx^2})] + bx^2(Ae^{-Bx^2})$

$= (-a)[-2B(1 - 2Bx^2)](Ae^{-Bx^2}) + bx^2(Ae^{-Bx^2})$

$= [(-a)[-2B(1 - 2Bx^2)] + bx^2](Ae^{-Bx^2})$

$= [(-a)[-2B(1 - 2Bx^2)] + bx^2]\,f$

$= cf,\ where\ c = (-a)[-2B(1 - 2Bx^2)] + bx^2$

To express A and B in terms of a, b, c, while c = 0.

$c = (-a)[-2B(1 - 2Bx^2)] + bx^2$

$4ax^2B^2 - 2aB - bx^2 = 0$

$$B = \frac{-(-2a)\pm\sqrt{(-2a)^2-4(4ax^2)(-bx^2)}}{2(4ax^2)}$$

$$B = \frac{2a\pm\sqrt{4a^2+16abx^4}}{8ax^2}$$

$$\int_{-\infty}^{\infty} Ae^{-Bx^2}dx = \frac{A\sqrt{\pi}}{2\sqrt{B}}\int\frac{2e^{-u^2}}{\sqrt{\pi}}du = \frac{A\sqrt{\pi}\,erf(x\sqrt{B})}{2\sqrt{B}}\Big|_{-\infty}^{\infty} = \frac{A\sqrt{\pi}}{\sqrt{B}}$$

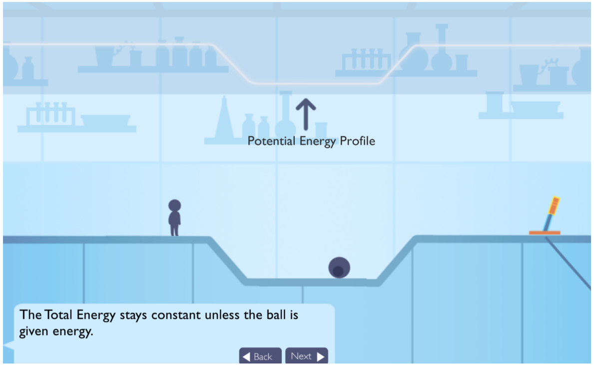
$$\frac{A\sqrt{\pi}}{\sqrt{B}} = 1 \rightarrow A = \sqrt{\frac{B}{\pi}}\ and\ B = A^2\pi$$

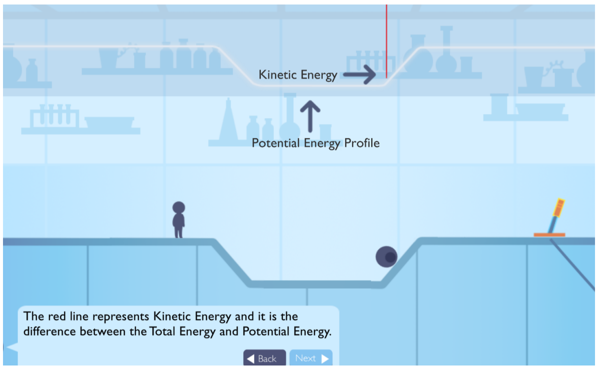
$$\therefore A = \sqrt{\frac{B}{\pi}} = [(\frac{2a\pm\sqrt{4a^2+16abx^4}}{8ax^2})(\pi^{-1})]^{\frac{1}{2}}$$

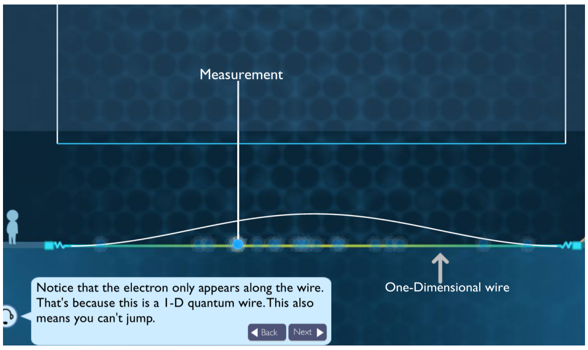
Week 8

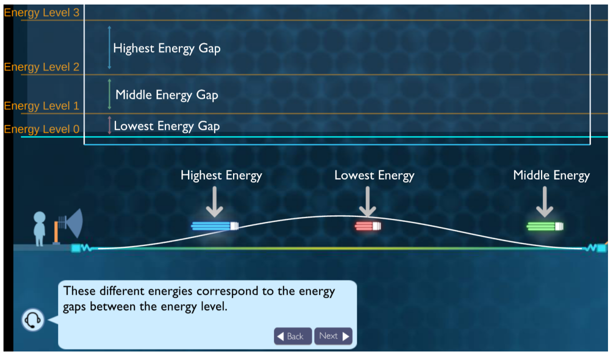
1. Play the Particle in a Box game here: https://learnqm.gatech.edu/ParticleInABox/index.html

- Take some screenshots of the classical and quantum parts of the game. What are the differences between what happens in these worlds?
- Based on the quantum game, what do you learn about the wavefunction?
- What part of the classical game was most difficult? What about the quantum game?









Difference between what happens in classical and quantum parts of the game

a. Classical world
   i. 2D, able to jump
   ii. Potential energy is directly related to height
   iii. When energy is given to the ball, total energy increases, so that the ball moves faster
b. Quantum world
   i. 1D quantum wire, unable to jump
   ii. Potential profile tells energy level and energy gap, is related to energy given to
   iii. When energy is given to the lamp, total energy increases, so that the wavefunction changes.

Based on the quantum game, I learnt things about wavefunction:

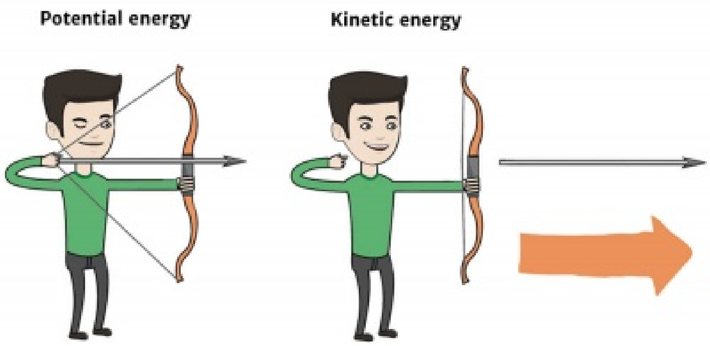
a. Maximum amplitude of wave = highest chance finding electron
b. Shape of wave function is determined by potential profile
c. The Color of photons determines energy. Lower wavelength means higher energy and vice-versa.
d. Number of nodes = energy level number

   Classical part is not difficult at all. But for the quantum game, it took me time to finish because the electron sparkles that can kill me are unpredictable.

2. Define, in your own words, the following terms:

- Kinetic energy
- Potential energy
- Hamiltonian
- Wavefunction
- Eigenvalue, eigenenergy (what are the differences between these, if any?)
- Eigenvector, eigenstate, eigenfunction (what are the differences between these, if any?)
- Superposition
- Normalization

- Kinetic energy and Potential energy
  Kinetic energy = energy of motion
  Potential energy = stored energy / energy from gravity
  E.g. The potential energy of the bowstring is transferred to the arrow it's fired. Arrow is then having kinetic energy.



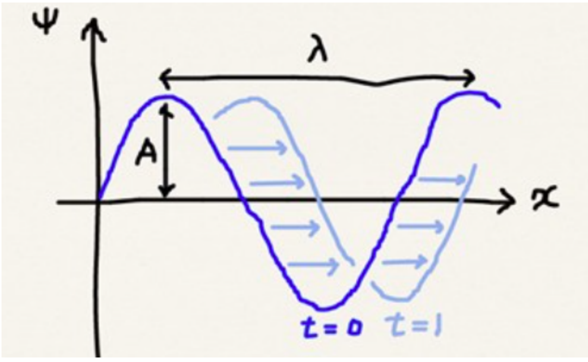
- Hamiltonian
  Kinetic energy operator
  $\hat{T} = \frac{\hat{p}^2}{2m} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$
  Potential energy operator
  $\hat{U} = U(x)$
  Hamiltonian operator
  $\hat{H} = \hat{T} + \hat{U}$

- <u>Wavefunction</u>

Each particle is represented by wavefunction $\psi(position,\ time)$.

$\psi(x, t)\ =\ A\ cos(\frac{2\pi}{\lambda}x\ -\ 2\pi vt)$

$\psi(x, t)\ =\ A\ sin(\frac{2\pi}{\lambda}x\ -\ 2\pi vt)$



By Euler's relation,

$e^{i\theta}\ =\ cos\theta\ +\ isin\theta$

$e^{x}\ =\ 1\ +\ x\ +\ \frac{x^2}{2!}\ +\ \frac{x^3}{3!}\ +\ \frac{x^4}{4!}...$

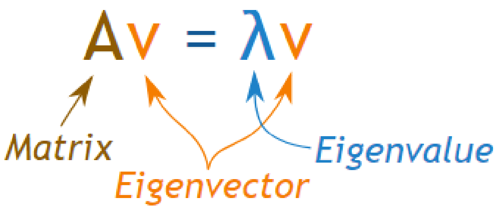
$cos\ x\ =\ 1\ -\ \frac{x^2}{2!}\ +\ \frac{x^4}{4!}\ -...$

$sin\ x\ =\ x\ -\ \frac{x^3}{3!}\ +\ \frac{x^5}{5!}\ -...$

We can use a function to represent a wave

$$\psi\ =\ e^{i(\frac{2\pi}{\lambda}x-2\pi vt)}$$

- <u>Eigenvalue, eigenenergy</u>



Operating on the wavefunction with the Hamiltonian produces the Schrodinger equation. $\widehat{H}\psi\ =\ E\psi$

From part b. Kinetic energy $\widehat{T}\ =\ \frac{\widehat{p}^2}{2m}\ =\ \frac{-\bar{h}^2}{2m}\frac{d^2}{dx^2}$

We can obtain the momentum operator $p\ =\ i\bar{h}\frac{d}{dx}$; $i\ =\ \sqrt{-\ 1}$

Act the momentum operator p on wave that differentiates with time:

$i\bar{h}\frac{d}{dt}\psi\ =\ i\bar{h}\frac{d}{dt}e^{i(\frac{2\pi}{\lambda}x-2\pi vt)}\ =\ i\bar{h}(-\ i2\pi v)e^{i(\frac{2\pi}{\lambda}x-2\pi vt)}\ =-\ i^2\frac{h}{2\pi}2\pi v\psi\ =\ hv\psi$

According to Planck, hv is energy $\rightarrow E\ \ =\ i\bar{h}\frac{d}{dt}$

$\therefore\ the\ wave\ is\ an\ eigenfunction\ with\ an\ energy\ eigenvalue\ (eigenenergy)\ of\ hv$

Substitute this into Schrodinger equation $\widehat{H}\psi\ =\ E\psi\ \rightarrow\ \widehat{H}\psi\ =\ i\bar{h}\frac{d\psi}{dt}$

To conclude, when operations produce specific values for the energy, it is eigenergy.

- <u>Eigenvector, eigenstate, eigenfunction</u>

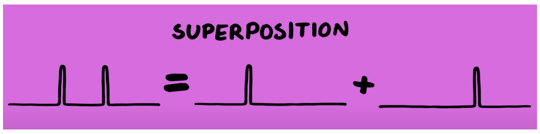
  $$= \underbrace{4}_{\textit{eigenvalue}} \underbrace{\begin{bmatrix} 1/2 \\ 1/2 \\ 1 \end{bmatrix}}_{\textit{eigenvector}}$$

  E.g. Eigenvector of matrix A = [1, 2, 3]. When multiplying matrix B by its eigenvector, the result is a scalar multiple of eigenvector.

  Eigenstate is a state of a quantum mechanical system that, when measured, always yields the same value.
  E.g. Eigenstate of electron → spin “up” / spin “down”
  E.g. Eigenstate of particle → represented by wave function
  E.g. Eigenstate of quantum mechanical system → used to calculate probabilities

  Eigenfunction is explained in part d already.

- <u>Superposition</u>
  Superposition is quantum phenomena where a particle can exist in two states at the same time.

- <u>Normalisation</u>
  Normalisation is scaling of wave function so that all the probabilities add to 1. A normalised wave function $\phi(x)$ would be said to be normalised if $\int [\phi(x)]^2 = 1$.

3. Normalize the following functions (that is, find A in terms of the other parameters of the function)

(i) $f(x) = Ae^{-ax^2}$

(ii) $f(x) = \begin{cases} A\sin(ax) & \text{for } 0 \le x \le L \\ 0 \text{ otherwise} \end{cases}$

(i) $\int [f(x)]^2 dx = \int [Ae^{-ax^2}]^2 dx = \int A^2 e^{-2ax^2} dx$

$$= \frac{A^2\sqrt{\pi}}{2^{\frac{3}{2}}\sqrt{a}} \int \frac{2e^{-u^2}}{\sqrt{\pi}} du, \ where\ u = \sqrt{2}\sqrt{a}x$$

$$= \frac{A^2\sqrt{\pi} erf(\sqrt{2a}x}{2^{\frac{3}{2}}\sqrt{a}} + C$$

$$\int_{-\infty}^{\infty} [f(x)]^2 dx = \frac{A^2\pi}{\sqrt{2a}} = 1$$

$$A = \frac{(2a)^{\frac{1}{4}}}{\sqrt{\pi}}$$

(ii) $f(x) = \begin{cases} sin(ax)\ for\ 0 \le x \le L \\ 0\ otherwise \end{cases}$

$$\int [f(x)]^2 dx = \begin{cases} \int_0^L sin^2(ax) dx \\ 0\ otherwise \end{cases}$$

$$\int [f(x)]^2 dx = \begin{cases} \int_0^L \frac{1}{2}(1 - cos\ (2ax)) dx \\ 0\ otherwise \end{cases}$$

$$\int [f(x)]^2 dx = \begin{cases} \frac{1}{2}\int_0^L 1 dx - \frac{1}{2}\int_0^L cos\ (2ax) dx \\ 0\ otherwise \end{cases}$$

$$\int [f(x)]^2 dx = \begin{cases} \left[\frac{x}{2} - \frac{sin2ax}{4a}\right]_0^L \\ 0\ otherwise \end{cases}$$

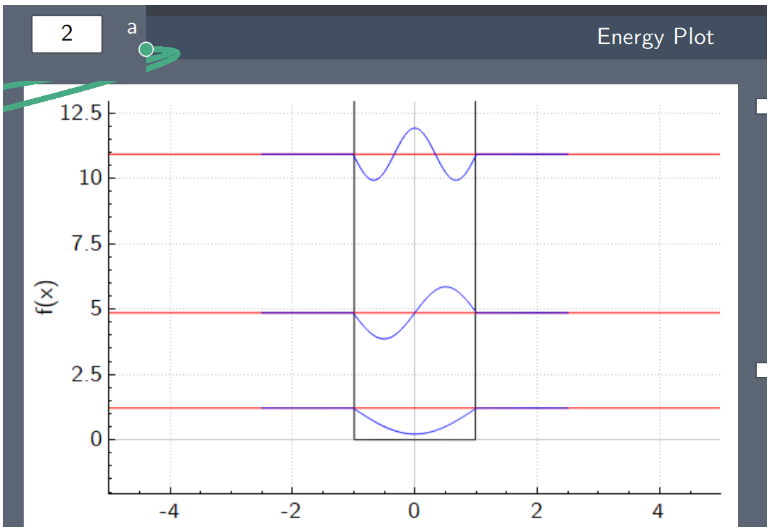
$$\int [f(x)]^2 dx = \begin{cases} \frac{L}{2} - \frac{sin(2La)}{4a} \\ 0\ otherwise \end{cases}$$

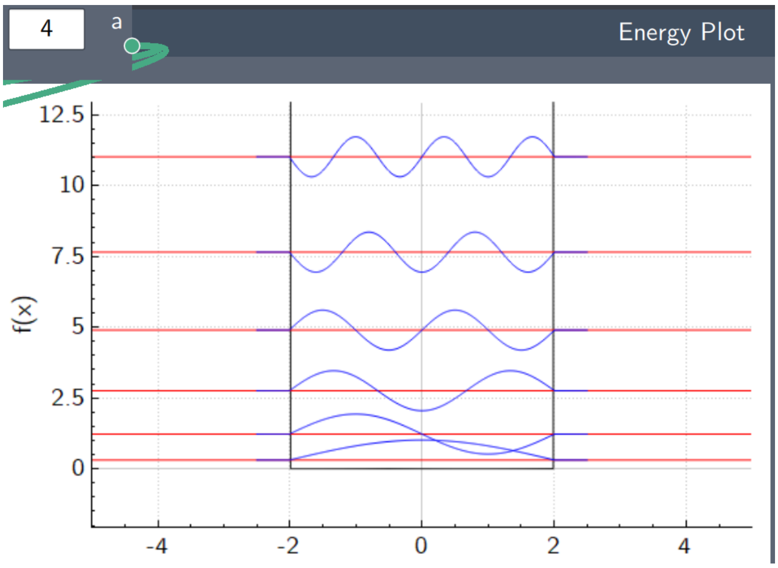
4. Download the Composer *infinite_well.flow* file from Blackboard. If you can't download Composer, you can work with a friend who can, but you should answer the questions below by yourself, in your own words.

- Find the potential box and change the value of a between 0.5 and 4. Write down and take screenshots: what do you notice? How is this similar to the waves on the string we covered earlier?

When we increase the value of a, the width of the well increases, also wave functions become denser to each other, meaning the energy gap becomes smaller.

The waves here are just like the waves on the string we covered earlier, wave at energy level 0 has 0 node, wave at energy level 1 has 1 node, and so on.





5. Download the Composer *finite_well.flow* file from Blackboard. If you can't download Composer, you can work with a friend who can, but you should answer the questions below by yourself, in your own words.

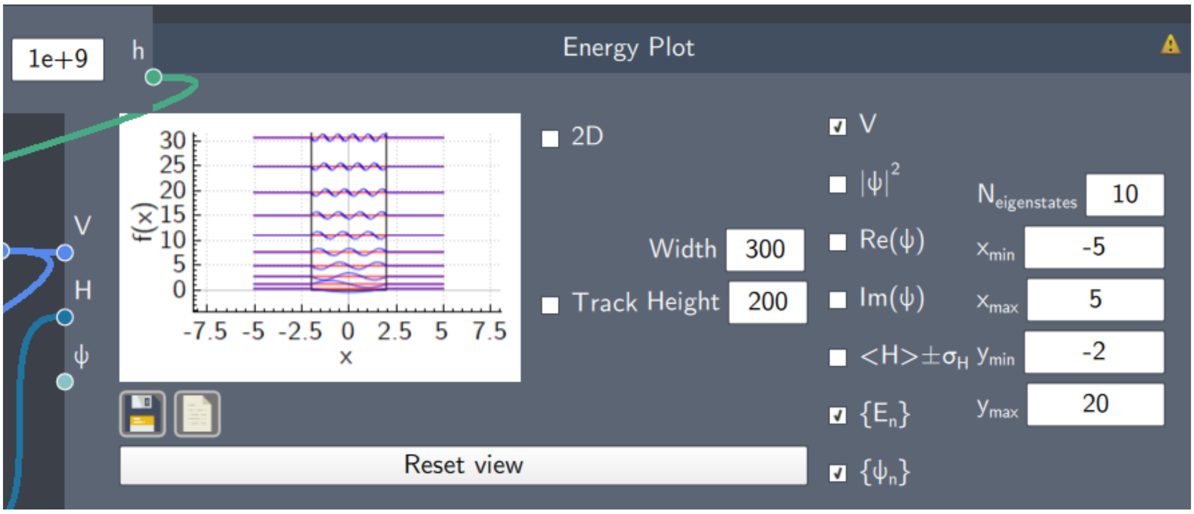
- Set the number of states to 10
- Explore values of h = 1e9 = 10^9, h = 10, h = 5, h = 2, h = 1. What changes? Take screenshots and write down in your own words.
- What is quantum about the states you see for small values of h? (Hint: can classical particles have probability to be in a wall?)
- For different values of h, how many states are bound inside the well? How many are outside the well? Make a plot (using, e.g., Excel)!

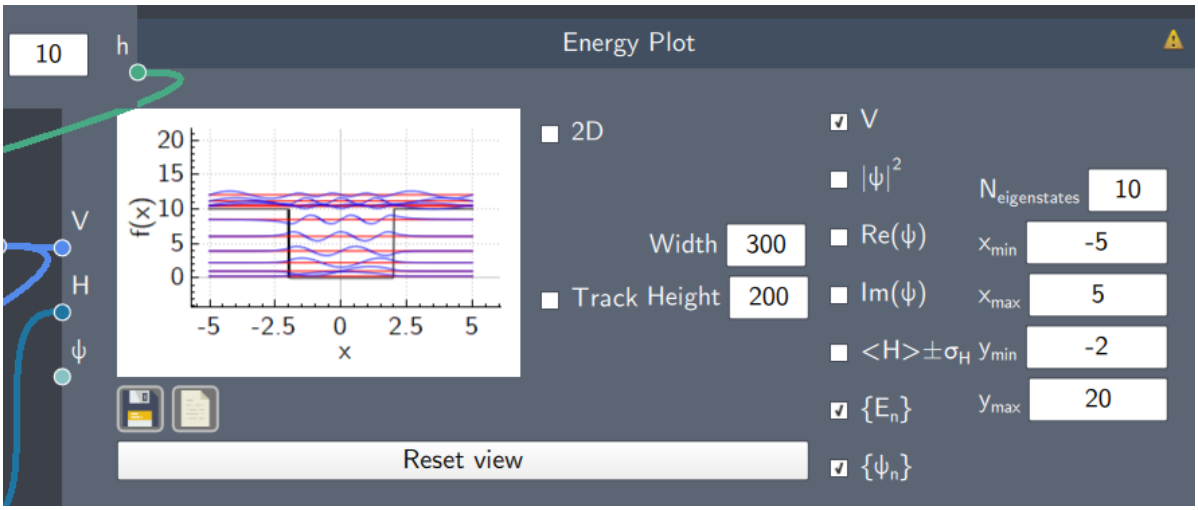
(i) When decrease value of h

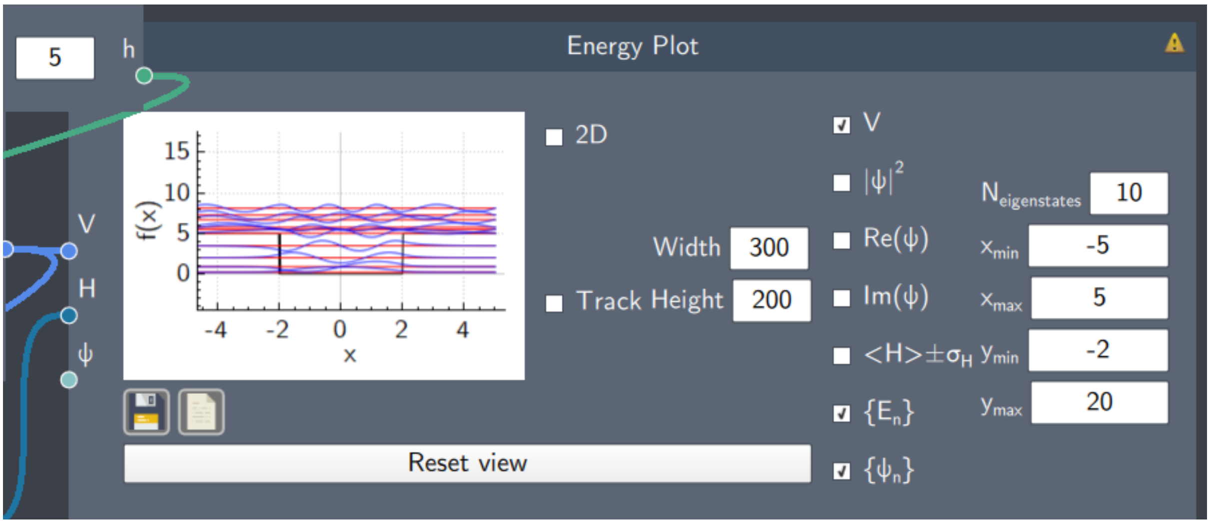
→ the maximum value of V, E_n and ψ_n decrease

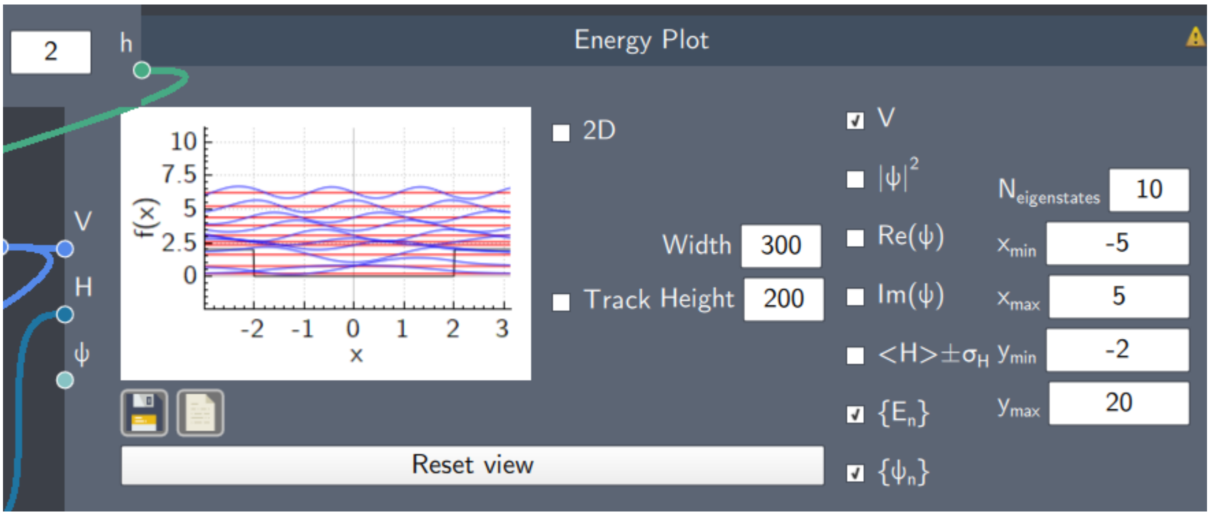
→ energy gap of E_n and ψ_n decrease

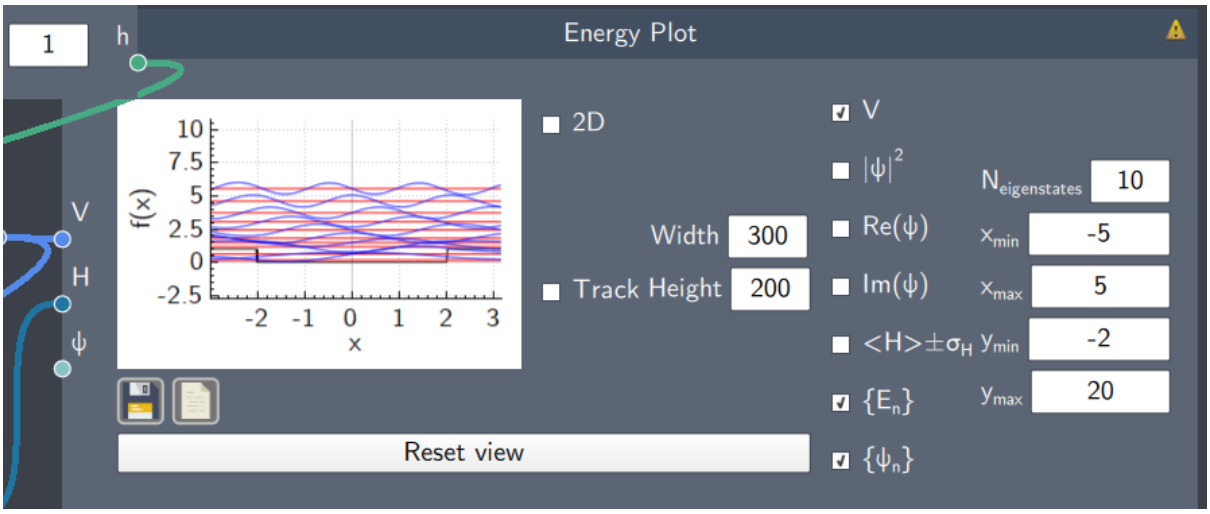
→ leakage, which means wavefunction can be spot beyond the well






5
h
Energy Plot
2D
Width 300
Track Height 200
Reset view
V
|ψ|²
Re(ψ)
Im(ψ)
<H>±σH
{En}
{ψn}
Neigenstates 10
xmin -5
xmax 5
ymin -2
ymax 20
H
ψ
f(x)
x


2
h
Energy Plot
2D
Width 300
Track Height 200
Reset view
V
|ψ|²
Re(ψ)
Im(ψ)
<H>±σH
{En}
{ψn}
Neigenstates 10
xmin -5
xmax 5
ymin -2
ymax 20
H
ψ
f(x)
x


1
h
Energy Plot
2D
Width 300
Track Height 200
Reset view
V
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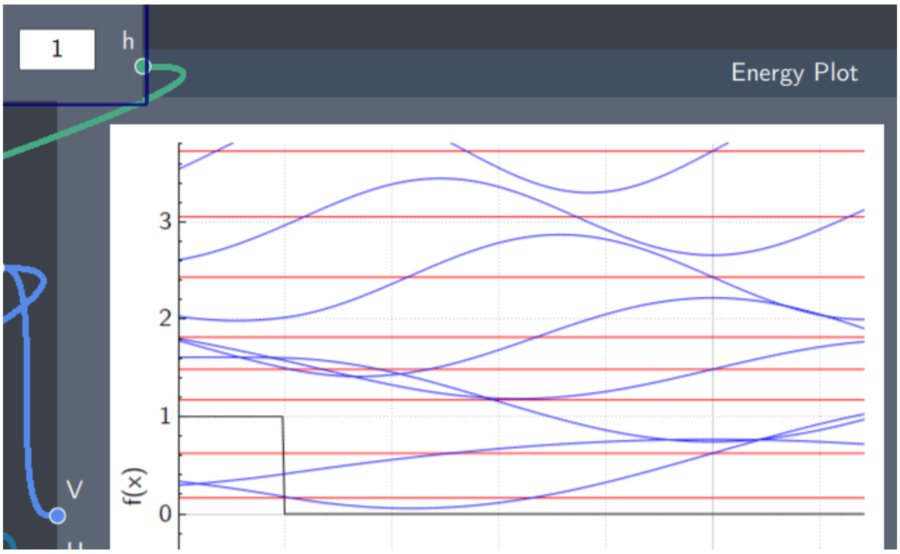
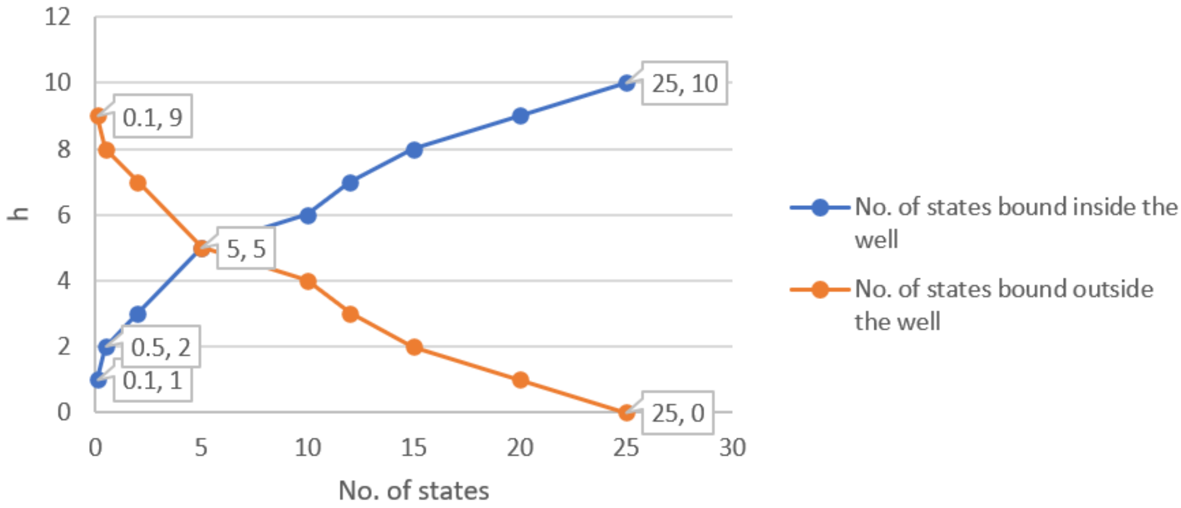
Re(ψ)
Im(ψ)
<H>±σH
{En}
{ψn}
Neigenstates 10
xmin -5
xmax 5
ymin -2
ymax 20
H
ψ
f(x)
x

(ii) When value of h is small, the well is smaller,



(iii)



6. For the infinite square well, if we label the ground state as $|0\rangle$, the first excited state as $|1\rangle$, and so on...what do the following states look like? You may check your answers with Composer, but you should try it on your own and draw this by hand!

(i) $|\psi\rangle = a(i|1\rangle - |2\rangle)$

(ii) $|\psi\rangle = b(|1\rangle + |2\rangle)$

(iii) $|\psi\rangle = c(|0\rangle - |1\rangle + i|2\rangle)$

(iv) $|\psi\rangle = d(1+i)|0\rangle$

(v) What are the values of a, b, c, and d in the equations above?

$|n\rangle = \sqrt{\frac{2}{L}}sin(\frac{n\pi x}{L})$, *where L is the width of well*

Suppose L = 2

$|0\rangle = sin(\frac{\pi x}{2})$

$|1\rangle = sin(\pi x)$

$|2\rangle = sin(\frac{3\pi x}{2})$

(i) $|\psi\rangle = a(i|1\rangle - |2\rangle)$

To normalise,

$\int |\psi|^2 dx = 1$

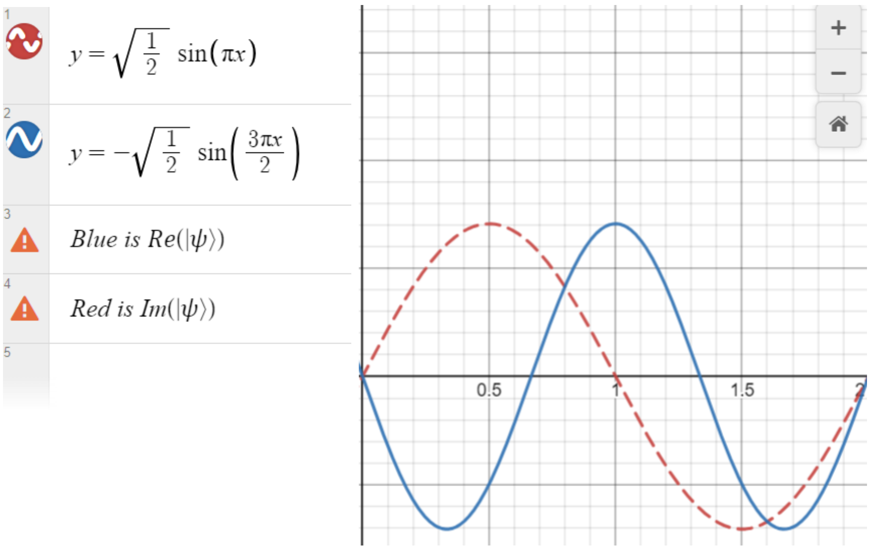
$\langle\psi|\psi\rangle = a(-i\langle 1| - \langle 2|)a(i|1\rangle - |2\rangle)$

$\langle\psi|\psi\rangle = |a|^2(-i^2\langle 1|1\rangle + i\langle 1|2\rangle - i\langle 2|1\rangle + \langle 2|2\rangle)$

$\langle\psi|\psi\rangle = |a|^2(1+1)$

$\langle\psi|\psi\rangle = 2|a|^2 = 1$

$a = \sqrt{\frac{1}{2}}$



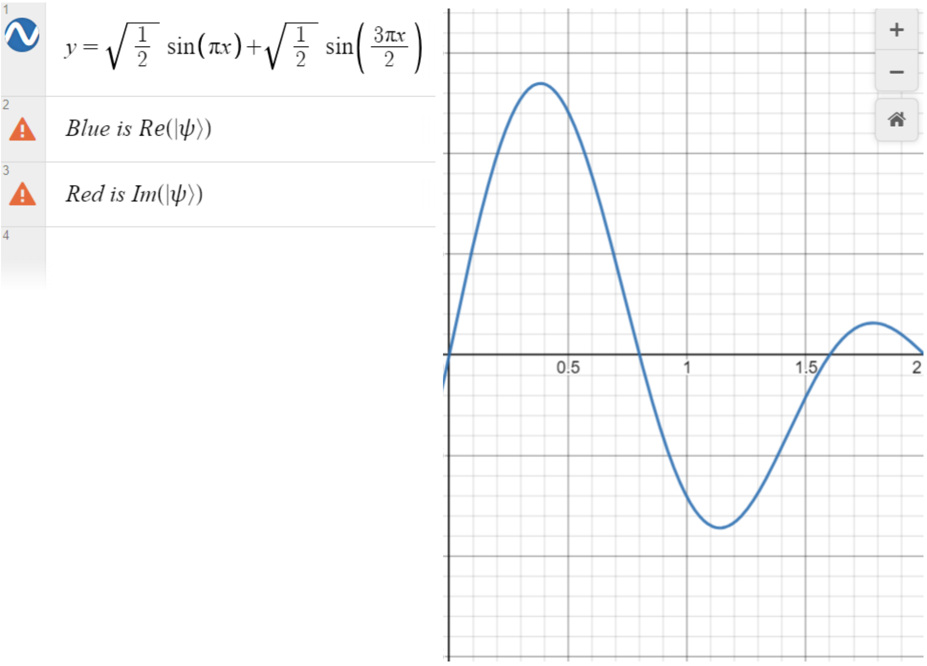
(ii) $|\psi\rangle = b(|1\rangle + |2\rangle)$

$\langle\psi|\psi\rangle = b(\langle 1| + \langle 2|)b(|1\rangle + |2\rangle)$

$\langle\psi|\psi\rangle = |b|^2(\langle 1|1\rangle + \langle 1|2\rangle + \langle 2|1\rangle + \langle 2|2\rangle)$

$\langle\psi|\psi\rangle = 2|b|^2 = 1$

$b = \sqrt{\frac{1}{2}}$



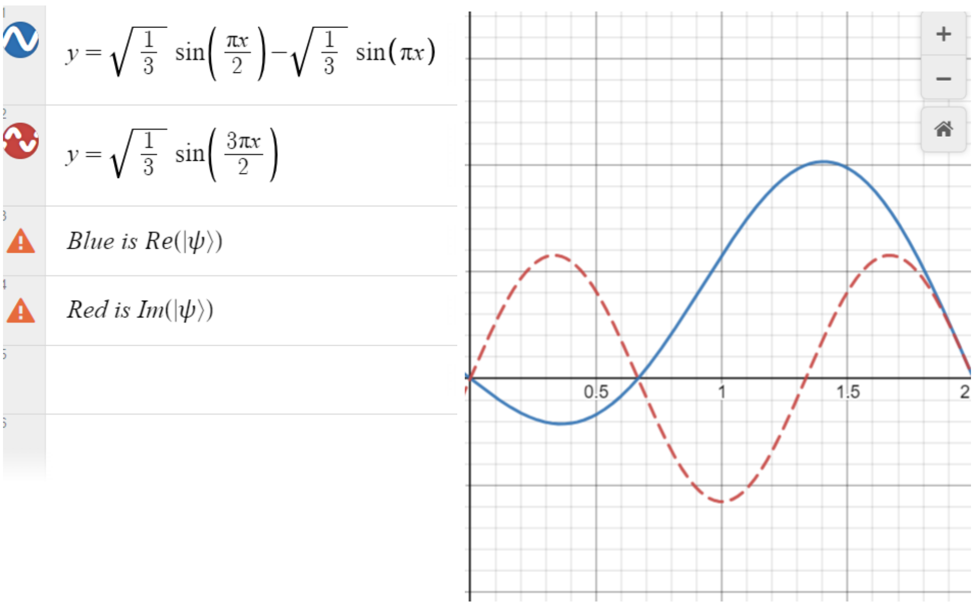
(iii) $|\psi\rangle = c(|0\rangle - |1\rangle + i|2\rangle)$

$\langle\psi|\psi\rangle = c(\langle 0| - \langle 1| - i\langle 2|)c(|0\rangle - |1\rangle + i|2\rangle)$

$\langle\psi|\psi\rangle = |c|^2(\langle 0|0\rangle + \langle 1|1\rangle - i^2\langle 2|2\rangle)$

$\langle\psi|\psi\rangle = 3|c|^2 = 1$

$c = \sqrt{\frac{1}{3}}$



(iv) $|\psi\rangle = d(1 + i)|0\rangle$

$e^{i\theta} = cos\theta + isin\theta$

$e^{\frac{i\pi}{4}} = \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}}i$

$\sqrt{2}e^{\frac{i\pi}{4}} = 1 + i$

$\langle\psi|\psi\rangle = |d(1 + i)|^2\langle 0|0\rangle$

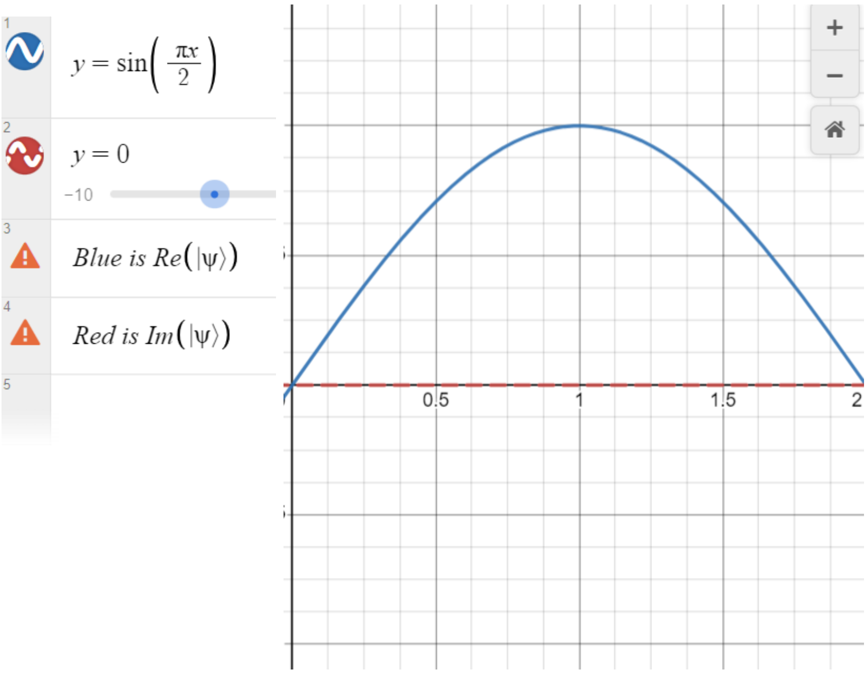
$\langle\psi|\psi\rangle = |d(\sqrt{2}e^{\frac{i\pi}{4}})|^2$

$\langle\psi|\psi\rangle = |d|^2 2e^{\frac{i\pi}{2}} = 1$

$|d|^2 = \frac{1}{2}e^{\frac{i\pi}{2}}$

$d = \frac{1}{\sqrt{2}}e^{\frac{-i\pi}{4}}$

$d(1 + i) = \frac{1}{\sqrt{2}}e^{\frac{i\pi}{4}}\sqrt{2}e^{\frac{-i\pi}{4}} = 1$



(v) Values of a, b, c, and d are calculated above already.

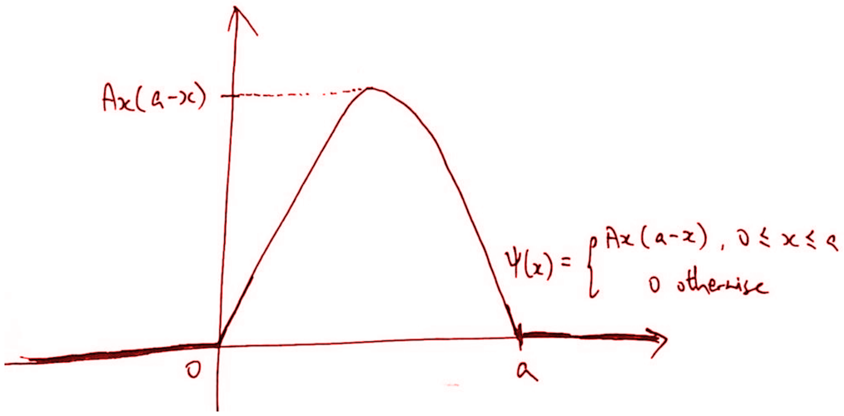
8. A particle in the infinite square well between 0 and a has the wavefunction

$$\psi(x) = \begin{cases} Ax(a-x), 0 \le x \le a \\ 0 \text{ otherwise} \end{cases}$$

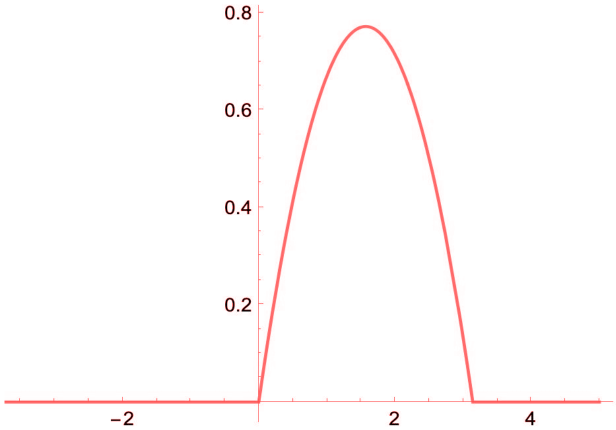
(i) Plot this wavefunction.

(ii) Determine the value of A.

(i)



To substitute $a = \pi$, $A = \sqrt{\frac{30}{a^5}}$



(ii)

$$\int_0^a [Ax(a-x)]^2\, dx = 1$$

$$\int_0^a A^2x^2(a^2 - 2ax + x^2) = 1$$

$$A^2a^2\int_0^a x^2 - 2A^2a\int_0^a x^3 + A^2\int_0^a x^4) = 1$$

$$[\frac{A^2a^2x^3}{3} - \frac{A^2ax^4}{2} + \frac{A^2x^5}{5}]_0^a = 1$$

$$\frac{10A^2a^5}{30} - \frac{15A^2a^5}{30} + \frac{6A^2a^5}{30}) = 1$$

$$\frac{A^2a^5}{30} = 1$$

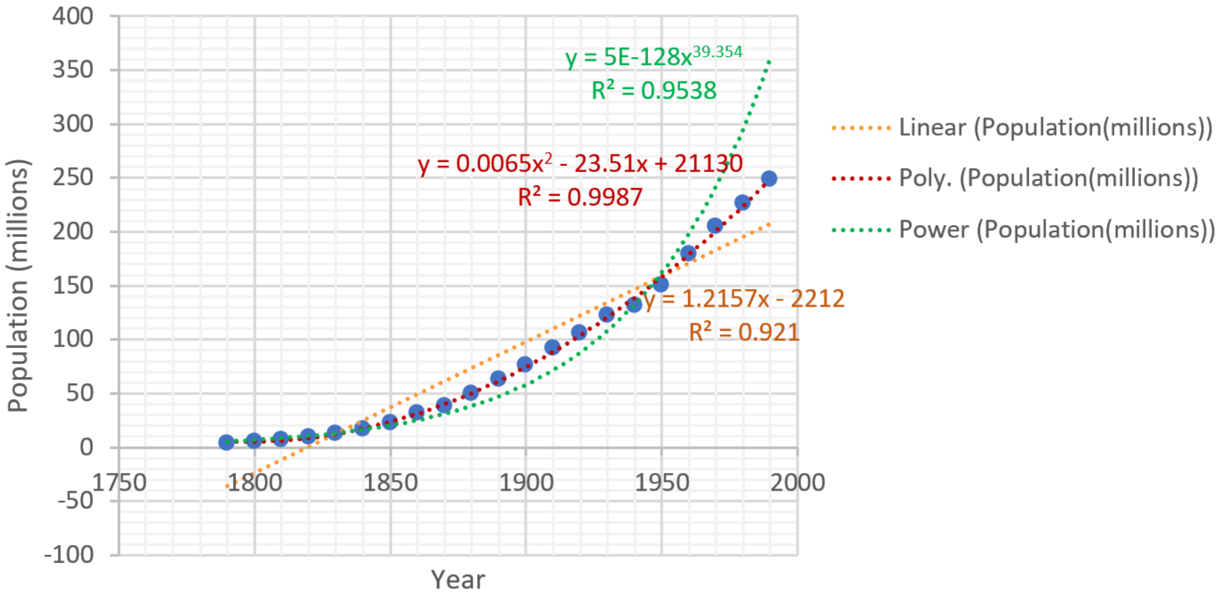
$$A = \sqrt{\frac{30}{a^5}}$$

9. In lecture, we looked (briefly) at a problem that requires us to do some curve fitting, which you'll explore in more detail on next week's problem sheet. You can use whatever computer plotting software you like to do the curve fitting in the next problem, but to be sure that everyone knows what to do, I would like you to go to https://engineerexcel.com/nonlinear-curve-fitting-in-excel-using-charts/ and plot the following data on a scatter chart. Then, fit the data to a line $f(x) = ax + b$, second-order polynomial (quadratic) $f(x) = ax^2 + bx + c$, and a power law $f(x) = ax^b + c$.

Find the parameters for each fit. Which fit is best? How do you know?

Data (this is the MATLAB census.mat, census data from 1790-1990 showing the growth in the US population):

Year	Population (millions)
1790	3.9000
1800	5.3000
1810	7.2000
1820	9.6000
1830	12.9000
1840	17.1000
1850	23.1000
1860	31.4000
1870	38.6000
1880	50.2000
1890	62.9000
1900	76.0000
1910	92.0000
1920	105.7000
1930	122.8000
1940	131.7000
1950	150.7000
1960	179.0000
1970	205.0000
1980	226.5000
1990	248.7000



Parameters are shown in the graph above.
Polynomial fits the best because it has the highest R-squared value, also by simply looking at the graph, the polynomial captures the trend of the data most accurately.

10. The ground state wavefunction in a harmonic well of frequency ω has wavefunction $\psi_0(x) = Ae^{-m\omega x^2/2\hbar}$.

(i) Normalize this wavefunction, that is, find A.

(ii) Applying the raising operator to this wavefunction, find the first excited state of the system. That is, find $\psi_1(x) = \hat{a}^\dagger\psi_0(x)$. Check—is this wavefunction normalized?

(iii) In the same way, find $\psi_2(x)$, the second excited state of the system. Is this wavefunction normalized?

(iv) Plot $\psi_0(x), \psi_1(x)$, and $\psi_2(x)$.

(iv) Check that $\psi_0(x), \psi_1(x)$, and $\psi_2(x)$ are orthogonal, that is, that $\int_{-\infty}^{\infty} dx\, \psi_\ell^*(x)\psi_n(x) = 0$ unless $\ell = n$.

(v) The expectation value of position, x, written as $\langle x\rangle$, is the place where we most expect to find our quantum particle, given that we measure its position. For a given wavefunction $\psi(x)$, we define $\langle x\rangle$ to be

$$\langle x\rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x) x \psi(x).$$

Find $\langle x\rangle$ for $\psi_0(x), \psi_1(x)$, and $\psi_2(x)$.

For most of the above, you will find the following to be useful (especially equation (11)): http://websites.umich.edu/~chem461/Gaussian%20Integrals.pdf

For all sub-questions, $\alpha = \frac{m\omega}{\hbar}$

(i) $\int [Ae^{\frac{-m\omega x^2}{2\hbar}}]^2 dx$

$= |A|^2 \int e^{-\alpha x^2} dx$

$$\because \quad \int_{-\infty}^{\infty} e^{-\alpha x^2}\, dx = \left(\frac{\pi}{\alpha}\right)^{1/2} \qquad (7)$$

$\therefore\ = |A|^2\sqrt{\frac{\pi}{\alpha}} = 1$

$A = (\frac{\alpha}{\pi})^{\frac{1}{4}} = (\frac{m\omega}{\pi\hbar})^{\frac{1}{4}}$

(ii) $a^{\dagger} = \sqrt{\frac{\alpha}{2}}(x - \frac{i}{m\omega}p)$ and $\psi_0(x) = (\frac{\alpha}{\pi})^{\frac{1}{4}} e^{\frac{-\alpha x^2}{2}}$

$$\psi_1(x) = a^{\dagger}\psi_0(x)$$

$$\psi_1(x) = \sqrt{\frac{\alpha}{2}}(x - \frac{i}{m\omega}p)(\frac{\alpha}{\pi})^{\frac{1}{4}} e^{\frac{-\alpha x^2}{2}}$$

$$\psi_1(x) = \sqrt{\frac{\alpha}{2}}(\frac{\alpha}{\pi})^{\frac{1}{4}}(x - \frac{\hbar}{m\omega}\frac{d}{dx})e^{\frac{-\alpha x^2}{2}}$$

$$\psi_1(x) = \sqrt{\frac{\alpha}{2}}(\frac{\alpha}{\pi})^{\frac{1}{4}}(x - \frac{1}{\alpha}\frac{d}{dx})e^{\frac{-\alpha x^2}{2}}$$

$$\psi_1(x) = \sqrt{\frac{\alpha}{2}}(\frac{\alpha}{\pi})^{\frac{1}{4}}(xe^{\frac{-\alpha x^2}{2}} - \frac{1}{\alpha}\frac{d}{dx}e^{\frac{-\alpha x^2}{2}})$$

$$\psi_1(x) = \sqrt{\frac{\alpha}{2}}(\frac{\alpha}{\pi})^{\frac{1}{4}}(xe^{\frac{-\alpha x^2}{2}} - \frac{1}{\alpha}(-\ \alpha xe^{\frac{-\alpha x^2}{2}}))$$

$$\psi_1(x) = \sqrt{\frac{\alpha}{2}}(\frac{\alpha}{\pi})^{\frac{1}{4}}(xe^{\frac{-\alpha x^2}{2}} + xe^{\frac{-\alpha x^2}{2}})$$

$$\psi_1(x) = \sqrt{\frac{\alpha}{2}}(\frac{\alpha}{\pi})^{\frac{1}{4}}(2xe^{\frac{-\alpha x^2}{2}})$$

$$\psi_1(x) = \sqrt{2\alpha}(\frac{\alpha}{\pi})^{\frac{1}{4}}(xe^{\frac{-\alpha x^2}{2}})$$

$$\int |\psi_1(x)|^2 dx = [\sqrt{2\alpha}(\frac{\alpha}{\pi})^{\frac{1}{4}}]^2 \int (xe^{\frac{-\alpha x^2}{2}})^2 dx$$

$$\int |\psi_1(x)|^2 dx = 2\alpha\sqrt{\frac{\alpha}{\pi}} \int x^2 e^{-\alpha x^2} dx$$

$$\int_{-\infty}^{\infty} x^2\, e^{-\alpha x^2}\, dx = \frac{\pi^{1/2}}{2\,\alpha^{3/2}} \qquad (9)$$

$$\int |\psi_1(x)|^2 dx = 2\alpha\sqrt{\frac{\alpha}{\pi}}\ \frac{\sqrt{\pi}}{2\alpha^{3/2}}$$

$$\int |\psi_1(x)|^2 dx = (\alpha)^{3/2}\ \frac{1}{\alpha^{3/2}}$$

$$\int |\psi_1(x)|^2 dx = 1$$

$\therefore$ *This wavefunction is normalised*

(iii) $\psi_n(x) = (a^\dagger)^n \psi_0(x)$

$\psi_2(x) = a^\dagger[a^\dagger \psi_0(x)]$

$\psi_2(x) = a^\dagger \psi_1(x)$

$\psi_2(x) = \sqrt{\frac{\alpha}{2}}(x - \frac{1}{\alpha}\frac{d}{dx})\sqrt{2\alpha}(\frac{\alpha}{\pi})^{\frac{1}{4}}(xe^{\frac{-\alpha x^2}{2}})$

$\psi_2(x) = \alpha(\frac{\alpha}{\pi})^{\frac{1}{4}}(x - \frac{1}{\alpha}\frac{d}{dx})(xe^{\frac{-\alpha x^2}{2}})$

$\psi_2(x) = \alpha(\frac{\alpha}{\pi})^{\frac{1}{4}}(x^2 e^{\frac{-\alpha x^2}{2}} - \frac{1}{\alpha}\frac{d}{dx}xe^{\frac{-\alpha x^2}{2}})$

$\psi_2(x) = \alpha(\frac{\alpha}{\pi})^{\frac{1}{4}}(x^2 e^{\frac{-\alpha x^2}{2}} - \frac{1}{\alpha}(e^{\frac{-\alpha x^2}{2}} - \alpha x e^{\frac{-\alpha x^2}{2}}))$

$\psi_2(x) = \alpha(\frac{\alpha}{\pi})^{\frac{1}{4}}(x^2 e^{\frac{-\alpha x^2}{2}} - \frac{1}{\alpha}e^{\frac{-\alpha x^2}{2}} + x^2 e^{\frac{-\alpha x^2}{2}})$

$\psi_2(x) = \alpha(\frac{\alpha}{\pi})^{\frac{1}{4}}(2x^2 e^{\frac{-\alpha x^2}{2}} - \frac{1}{\alpha}e^{\frac{-\alpha x^2}{2}})$

$\int|\psi_2(x)|^2 dx = \alpha^2\sqrt{\frac{\alpha}{\pi}}\int(2x^2 e^{\frac{-\alpha x^2}{2}} - \frac{1}{\alpha}e^{\frac{-\alpha x^2}{2}})^2 dx$

$\int|\psi_2(x)|^2 dx = \alpha^2\sqrt{\frac{\alpha}{\pi}}\int(2x^2 e^{\frac{-\alpha x^2}{2}} - \frac{1}{\alpha}e^{\frac{-\alpha x^2}{2}})^2 dx$

$\int|\psi_2(x)|^2 dx = \alpha^2\sqrt{\frac{\alpha}{\pi}}\int 4x^4 e^{-\alpha x^2} - \frac{4}{\alpha}x^2 e^{-\alpha x^2} + \frac{1}{\alpha^2}e^{-\alpha x^2} dx$

$\int|\psi_2(x)|^2 dx = \alpha^2\sqrt{\frac{\alpha}{\pi}}(4\int x^4 e^{-\alpha x^2} dx - \frac{4}{\alpha}\int x^2 e^{-\alpha x^2} dx + \frac{1}{\alpha^2}\int e^{-\alpha x^2} dx)$

$\int|\psi_2(x)|^2 dx = \alpha^2\sqrt{\frac{\alpha}{\pi}}(4\frac{3\sqrt{\pi}}{4\alpha^{5/2}} - \frac{4}{\alpha}\frac{\sqrt{\pi}}{2\alpha^{3/2}} + \frac{1}{\alpha^2}\frac{\sqrt{\pi}}{\sqrt{\alpha}})$

$\int|\psi_2(x)|^2 dx = \alpha^2\sqrt{\frac{\alpha}{\pi}}\frac{3\sqrt{\pi}}{\alpha^{5/2}} - \alpha^2\sqrt{\frac{\alpha}{\pi}}\frac{2}{\alpha}\frac{\sqrt{\pi}}{\alpha^{3/2}} + \alpha^2\sqrt{\frac{\alpha}{\pi}}\frac{1}{\alpha^2}\frac{\sqrt{\pi}}{\sqrt{\alpha}})$

$\int|\psi_2(x)|^2 dx = 3 - 2 + 1$

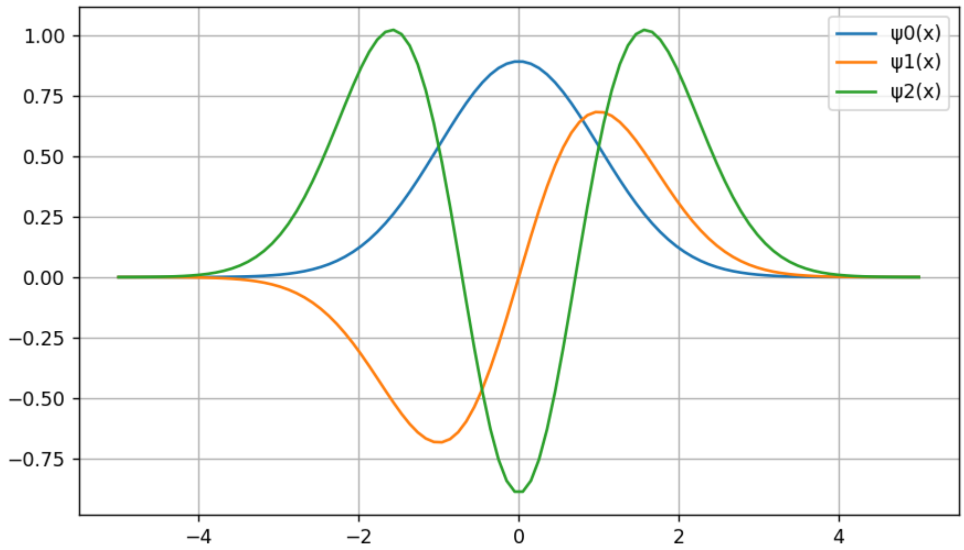
$\int|\psi_2(x)|^2 dx = 2 \neq 1$

∵ We use the same way instructed in (b), which normalisation constant is not added, and we see $\int|\psi_2(x)|^2 dx \neq 1$

∴ This wavefunction is not normalised

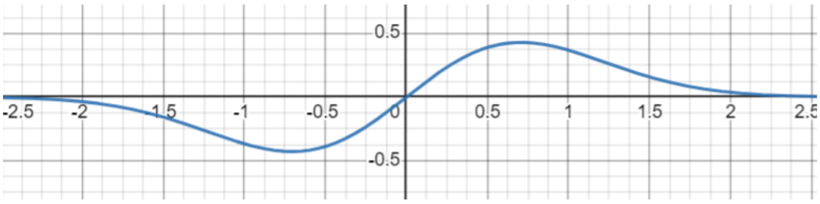
(iv) In order to plot the graph, substitute m=1, ω = 2, and ħ = 1.
And then plot by python,

```
psi_0 = ((2 / np.pi) ** (1 / 4)) * np.exp(-x ** 2 / 2)
psi_1 = np.sqrt(4 / np.pi) * x * np.exp(-x ** 2 / 2)
psi_2 = ((2 / np.pi) ** (1 / 4)) * (2 * x ** 2 * np.exp(-x ** 2 / 2) -
np.exp(-x ** 2 / 2))
```



(v) $\int \psi_0^*(x)\psi_1(x)dx = \int (\frac{\alpha}{\pi})^{\frac{1}{4}} e^{\frac{-\alpha x^2}{2}} \sqrt{2\alpha}(\frac{\alpha}{\pi})^{\frac{1}{4}}(xe^{\frac{-\alpha x^2}{2}})dx$

$\int \psi_0^*(x)\psi_1(x)dx = \sqrt{\frac{2}{\pi}}\alpha \int xe^{-\alpha x^2} dx$



The integral vanishes because the total area of the function above the x-axis cancels the (negative) area below it.

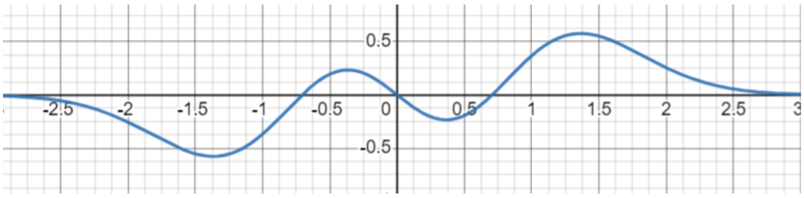
$\int \psi_0^*(x)\psi_1(x)dx = 0$

$\int \psi_1^*(x)\psi_2(x)dx = \int \sqrt{2\alpha}(\frac{\alpha}{\pi})^{\frac{1}{4}}(xe^{\frac{-\alpha x^2}{2}})\alpha(\frac{\alpha}{\pi})^{\frac{1}{4}}(2x^2 e^{\frac{-\alpha x^2}{2}} - \frac{1}{\alpha}e^{\frac{-\alpha x^2}{2}})dx$

$\int \psi_1^*(x)\psi_2(x)dx = \int \sqrt{\frac{2}{\pi}}\alpha^2(xe^{-\alpha x^2})(2x^2 - \frac{1}{\alpha})dx$

$\int \psi_1^*(x)\psi_2(x)dx = \sqrt{\frac{2}{\pi}}\alpha \int (xe^{-\alpha x^2})(2\alpha x^2 - 1)dx$

The integral vanishes because the total area of the function above the x-axis cancels the (negative) area below it.



Area between two will be 0.

$\int \psi_1^*(x)\psi_2(x)dx = 0$

$\int \psi_0^*(x)\psi_2(x)dx = \int (\frac{\alpha}{\pi})^{\frac{1}{4}} e^{\frac{-\alpha x^2}{2}} \alpha(\frac{\alpha}{\pi})^{\frac{1}{4}}(2x^2 e^{\frac{-\alpha x^2}{2}} - \frac{1}{\alpha}e^{\frac{-\alpha x^2}{2}})dx$

$\int \psi_0^*(x)\psi_2(x)dx = \alpha\sqrt{\frac{\alpha}{\pi}}\int (2x^2 e^{-\alpha x^2} - \frac{1}{\alpha}e^{-\alpha x^2})dx$

$\int \psi_0^*(x)\psi_2(x)dx = \sqrt{\frac{\alpha}{\pi}}\int (2\alpha x^2 e^{-\alpha x^2} - e^{-\alpha x^2})dx$

$\int \psi_0^*(x)\psi_2(x)dx = \sqrt{\frac{\alpha}{\pi}}\int (2\alpha\frac{\pi^{1/2}}{2\alpha^{3/2}} - \frac{\pi^{1/2}}{\alpha^{1/2}})dx$

$\int \psi_0^*(x)\psi_2(x)dx = 0$

$\therefore \psi_0(x),\ \psi_1(x)$ *and* $\psi_2(x)$ *are orthogonal.*

(vi) To find ⟨x⟩ for ψ0(x)

$$\langle x\rangle = \int \psi_0^*(x) x \psi_0(x) dx$$

$$\langle x\rangle = \int x |(\frac{\alpha}{\pi})^{\frac{1}{4}} e^{\frac{-\alpha x^2}{2}}|^2 dx$$

$$\langle x\rangle = \sqrt{\frac{\alpha}{\pi}} \int x e^{-\alpha x^2} dx$$

$$\langle x\rangle = 0$$

To find ⟨x⟩ for ψ1(x)

$$\langle x\rangle = \int \psi_1^*(x) x \psi_1(x) dx$$

$$\langle x\rangle = \int x |\sqrt{2\alpha}(\frac{\alpha}{\pi})^{\frac{1}{4}} (x e^{\frac{-\alpha x^2}{2}})|^2 dx$$

$$\langle x\rangle = 2\alpha\sqrt{\frac{\alpha}{\pi}} \int x^3 e^{-\alpha x^2} dx$$

$$\langle x\rangle = 0$$

To find ⟨x⟩ for ψ2(x)

$$\langle x\rangle = \int \psi_2^*(x) x \psi_2(x) dx$$

$$\langle x\rangle = \int x |\alpha(\frac{\alpha}{\pi})^{\frac{1}{4}} (2x^2 e^{\frac{-\alpha x^2}{2}} - \frac{1}{\alpha} e^{\frac{-\alpha x^2}{2}})|^2 dx$$

$$\langle x\rangle = \alpha^2\sqrt{\frac{\alpha}{\pi}} \int [4x^5 e^{-\alpha x^2} - 2(2x^3 e^{\frac{-\alpha x^2}{2}})(\frac{1}{\alpha} e^{\frac{-\alpha x^2}{2}}) + \frac{1}{\alpha^2} x e^{-\alpha x^2}] dx$$

$$\langle x\rangle = 0$$

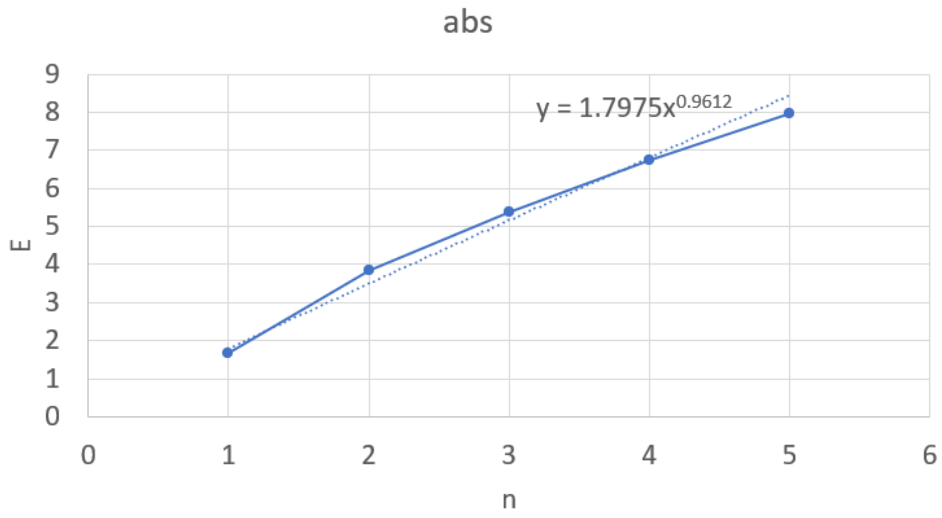
Week 9

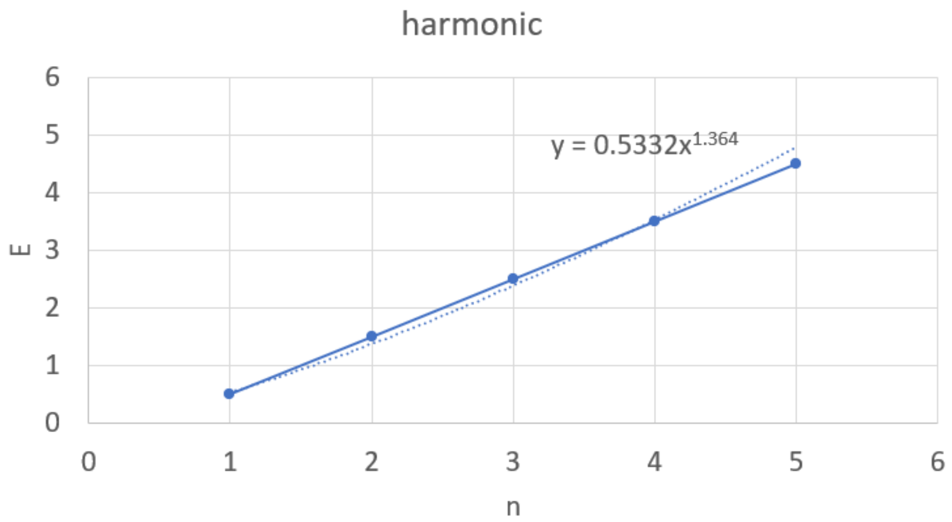
1. In the lecture, we looked at four different potentials: the quartic well $V(x) \propto x^4$, the harmonic well $V(x) \propto x^2$, the absolute value potential $V(x) \propto |x|$, and the infinite square well, $V(x) \propto x^\infty$. In the Composer files corresponding to this potential, you can find the numbers corresponding to the first five energy levels. You should use the tools you developed as a part of Problem 9 and fit these values to a power law, $E(n) = an^b$, where $E(n)$ is the energy at level n.

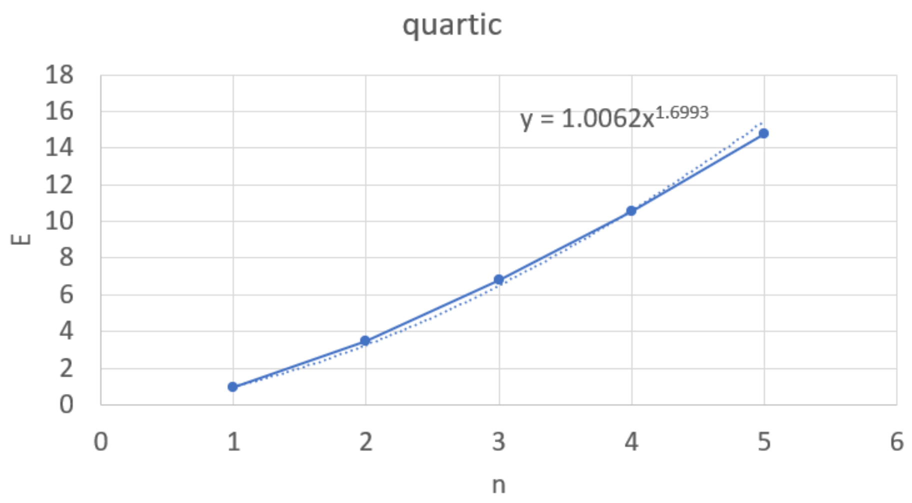
(i) What is b for each of these potentials?

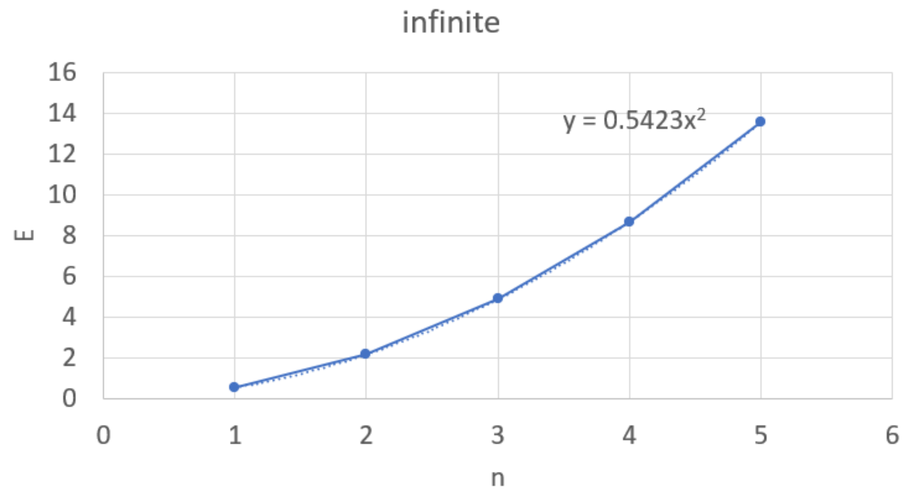
(ii) If you were designing a qubit (i.e., isolating a two-level system), which potential(s) would you want to use? Which would you NOT want to use?

(i) $E(n) = an^b$. Value of b for each potential is shown in the following plots.
Value of b for abs is 0.9612, for harmonic is 1.364, for quartic is 1.6693, for infinite is 2.









(ii) If I was designing a qubit (i.e., isolating a two - level system), I would use potentials that provide energy levels that can be distinguishable from each other. I would choose Quartic and Infinite because energy separation is different. I would not choose Abs and harmonic because their energy separation is almost identical.

2. Open the *band_structure.flow* file.

(i) You should see one well. How many bound states are in this well? What happens to the states that are outside of this well?

(ii) Now add more wells by changing which nodes are connected to the V nodes of the “Hamiltonian” and “Energy Plot” nodes (be sure to connect both!) and answer the following questions:

(iii) How do the energy levels of the system change as you add wells?

(iv) For the number of wells $N = 1, 2, 3, 4,$ and 5, write down and plot the energies of the first $4N$ levels. What do you notice?

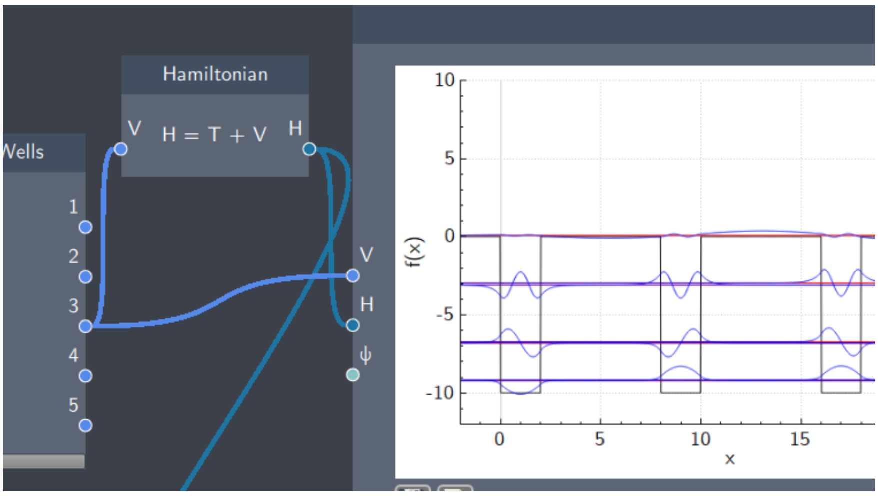
(v) What happens to the width of the bands as you change the well separation? Take some screenshots!

(vi) What do you think happens if the number of wells goes to infinity?

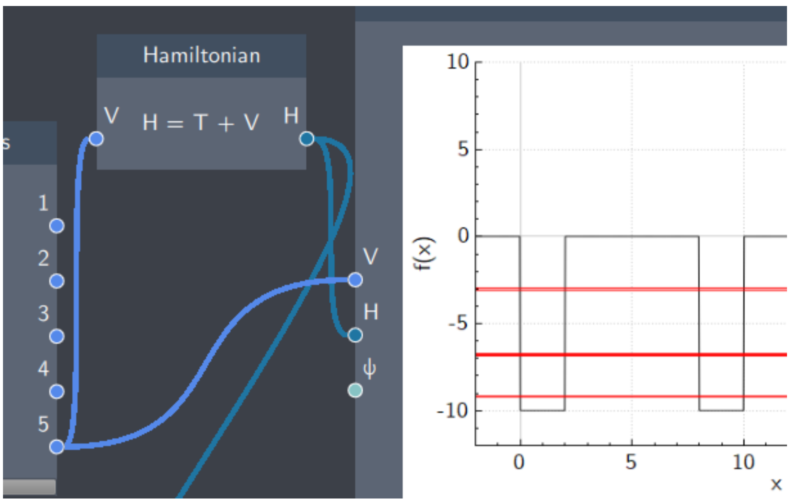
(vii) Which wells would you consider to be the valence bands? Which are the conduction bands?

(i) Three bound states in the well. They oscillate within the well, but decay away outside the well.

(ii)

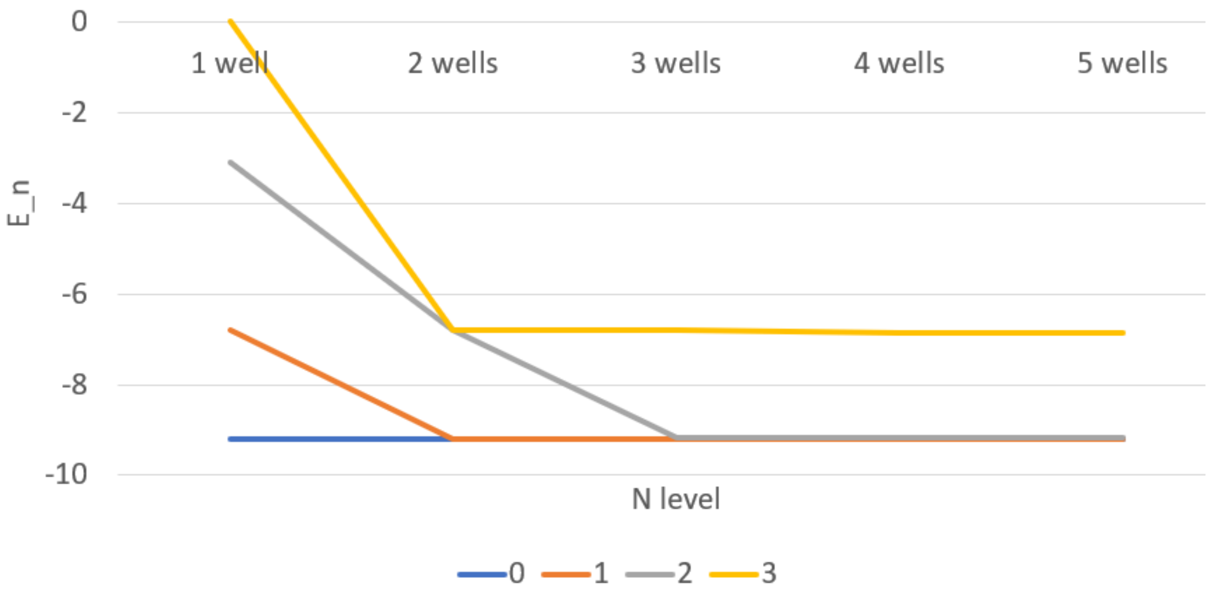


(iii) When I add more wells, energy levels become denser toward the bottom of the well.



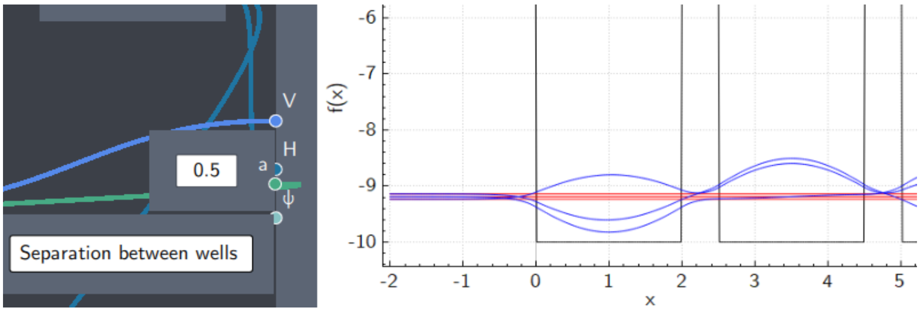
(iv) For the number of wells N = 1 , 2 , 3 , 4 , and 5, the energies of the first 4 N levels were recorded and plotted by excel as shown below.

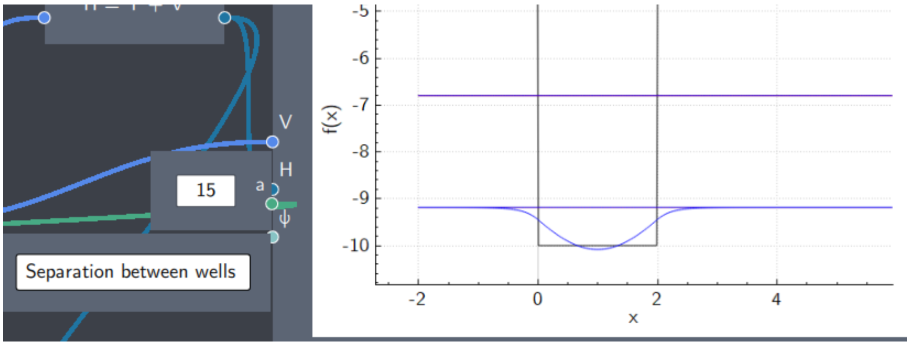
	E_n				
N level	1 well	2 wells	3 wells	4 wells	5 wells
0	-9.18447515	-9.18448	-9.18448	-9.18448	-9.18448
1	-6.79495445	-9.18448	-9.18448	-9.18448	-9.18448
2	-3.0845572	-6.79495	-9.16679	-9.16679	-9.16679
3	0.00902514	-6.79495	-6.79495	-6.85037	-6.85037

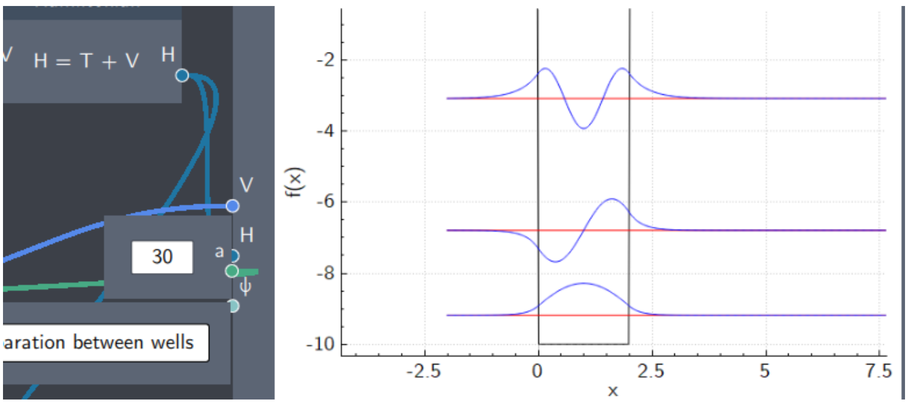


I noticed that energies decrease dramatically in the beginning as we increase the number of wells. However, once the number of wells reaches three, further increases in the number of wells result in only minor and barely perceptible changes in the energy levels.

(v) I set the eigenstates to be 3. I changed the well separation from 0.5 to 15, 15 to 30. And I observed that, when the separation between wells is larger, the width of the bands become closer.







(vi) I think all energy levels will be far apart at a high value for the number of wells, but it may reach a maximum point at a certain point. If the number of wells goes infinity, the energy levels won't go further apart after reaching a certain point.

(vii) I am quite confused answering this question.I know the width we mentioned in the above subquestion is bandgap. And bandgap is the energy difference between highest energy level and lowest energy level. The higher energy level region is where the conduction band is, while the lower energy level region is where the valence band is.

3. In lecture, we talked about the time-dependence of wavefunctions, and all we want you to do in this problem is to go over some of the maths yourself. Show, in general, that if you have a function $\psi(t)$ obeying a differential equation of the form $i\hbar \frac{d\psi}{dt} = E\psi$ for some E, then $\psi(t) = e^{-iEt/\hbar}\psi(0)$, where $\psi(0)$ is our initial condition.

$i\hbar \frac{d\psi}{dt} = E\psi$

$\frac{1}{\psi} d\psi = \frac{-iE}{\hbar} dt$

Integrate both sides,,

$\int \frac{1}{\psi} d\psi = \int \frac{-iE}{\hbar} dt$

$\ln \psi = \frac{-iEt}{\hbar} + C$

Exponentiate both sides,,

$\psi(x, t) = e^{-iEt/\hbar + C}$

$\psi(x, t) = e^{-iEt/\hbar} e^{C}$

Use constant waveform $\psi(x, 0)$ for e^{C},,

$\psi(0, t) = e^{-iEt/\hbar} \psi(0)$

4. If you have a wavefunction $\psi(x, t=0) = \psi_0(x)$, where $\psi_0(x)$ is the (real) ground state wavefunction of the harmonic oscillator with energy $E_0 = \hbar\omega/2$ that we discussed in Week 8, how do the real and imaginary parts of $\psi(x,t)$ change with time? How does $|\psi(x,t)|^2$ change? Show your work, particularly for $t = \frac{\pi}{2E_0}, \frac{\pi}{E_0}$, and $\frac{2\pi}{E_0}$. You can check your answer in Composer! (Use *single_well.flow*).

$\psi(x, t = 0) = \psi_0(x)$, where $\psi_0(x)$ is the (real) ground state wavefunction of the harmonic oscillator with energy $E_0 = \hbar\omega/2$.

How do the real and imaginary parts of $\psi(x, t)$ change with time will be explained by calculation below.

Now, $\psi(x, t) = e^{-iEt/\hbar} e^{C}$ can be written as $\psi_0(x, t) = e^{-iE_0 t/\hbar}\psi_0(x)$.

To substitute E_0, can be written as $\psi(x, t) = e^{-i\frac{\omega}{2}t}\psi_0(x)$.

$e^{-i\frac{\omega}{2}t} = cos(\frac{\omega}{2}t) - isin(\frac{\omega}{2}t)$

For $t = \frac{\pi}{2E_0}$,

$cos(\frac{\omega}{2}\frac{\pi}{2E_0}) - isin(\frac{\omega}{2}\frac{\pi}{2E_0}) = cos(\frac{\omega}{2}\frac{2\pi}{2\hbar\omega}) - isin(\frac{\omega}{2}\frac{2\pi}{2\hbar\omega})$

Suppose $\hbar = 1$,

$= cos(\frac{\pi}{2}) - isin(\frac{\pi}{2})$

For $t = \frac{\pi}{E_0}$,

$cos(\frac{\omega}{2}\frac{\pi}{E_0}) - isin(\frac{\omega}{2}\frac{\pi}{E_0}) = cos(\frac{\omega}{2}\frac{2\pi}{\hbar\omega}) - isin(\frac{\omega}{2}\frac{2\pi}{\hbar\omega})$

Suppose $\hbar = 1$,

$= cos(\pi) - isin(\pi)$

For $t = \frac{2\pi}{E_0}$,

$cos(\frac{\omega}{2}\frac{2\pi}{E_0}) - isin(\frac{\omega}{2}\frac{2\pi}{E_0}) = cos(\frac{\omega}{2}\frac{4\pi}{\hbar\omega}) - isin(\frac{\omega}{2}\frac{4\pi}{\hbar\omega})$

Suppose $\hbar = 1$,

$= cos(2\pi) - isin(2\pi)$

$|\psi_0(x,t)|^2 = |e^{-i\frac{\omega}{2}t}|^2 |\psi_0(x)|^2 = |\psi_0(x)|^2$

For $t = \frac{\pi}{2E_0}$,

$= |\psi_0(x)|^2$

For $t = \frac{\pi}{E_0}$,

$= |\psi_0(x)|^2$

For $t = \frac{2\pi}{E_0}$,

$= |\psi_0(x)|^2$

∴ Real and imaginary parts of $\psi_0(x,t)$ time dependent and $|\psi_0(x,t)|^2$ are time independent.

5. How does your answer to Problem 4 change if we instead use the $\psi(x, t = 0) = \psi_1(x)$, where $\psi_1(x)$ is the (real) first excited state wavefunction of the harmonic oscillator with energy $E_1 = 3\hbar\omega/2$? Show your work, particularly for $t = \frac{\pi}{2E_1}, \frac{\pi}{E_1}$, and $\frac{2\pi}{E_1}$.

$\psi_1(x, t = 0) = \psi_1(x)$, where $\psi_1(x)$ is the (real) first state wavefunction of the harmonic oscillator with energy $E_1 = 3\hbar\omega/2$.

$\psi_1(x, t) = e^{-i\frac{3\omega}{2}t}\psi_1(x)$.

$e^{-i\frac{3\omega}{2}t} = cos(\frac{3\omega}{2}t) - isin(\frac{3\omega}{2}t)$

For $t = \frac{\pi}{2E_1}$,

$cos(\frac{3\omega}{2}\frac{\pi}{2E_1}) - isin(\frac{3\omega}{2}\frac{\pi}{2E_1}) = cos(\frac{3\omega}{2}\frac{2\pi}{6\hbar\omega}) - isin(\frac{3\omega}{2}\frac{2\pi}{6\hbar\omega})$

Suppose $\hbar = 1$,

$= cos(\frac{\pi}{2}) - isin(\frac{\pi}{2})$

For $t = \frac{\pi}{E_1}$,

$cos(\frac{3\omega}{2}\frac{\pi}{E_1}) - isin(\frac{3\omega}{2}\frac{\pi}{E_1}) = cos(\frac{3\omega}{2}\frac{2\pi}{3\hbar\omega}) - isin(\frac{3\omega}{2}\frac{2\pi}{3\hbar\omega})$

Suppose $\hbar = 1$,

$= cos(\pi) - isin(\pi)$

For $t = \frac{2\pi}{E_1}$,

$cos(\frac{3\omega}{2}\frac{2\pi}{E_1}) - isin(\frac{3\omega}{2}\frac{2\pi}{E_1}) = cos(\frac{3\omega}{2}\frac{4\pi}{3\hbar\omega}) - isin(\frac{3\omega}{2}\frac{4\pi}{3\hbar\omega})$

Suppose $\hbar = 1$,

$= cos(2\pi) - isin(2\pi)$

$|\psi(x,t)|^2 = |e^{-i\frac{3\omega}{2}t}|^2|\psi_1(x)|^2 = |\psi_1(x)|^2.$

For $t = \frac{\pi}{2E_1}$,

$= |\psi_1(x)|^2$

For $t = \frac{\pi}{E_1}$,

$= |\psi_1(x)|^2$

For $t = \frac{2\pi}{E_1}$,

$= |\psi_1(x)|^2$

$\therefore$ Real and imaginary parts of $\psi_1(x,t)$ time dependent and $|\psi_1(x,t)|^2$ are time independent.

6. Given (for an eigenstate)

$$\psi_e(x,t) = e^{-iEt/\hbar}\psi(x,0)$$

As well as (for a superposition)

$$\psi_s(x,t) = \frac{1}{\sqrt{2}}\left(e^{-iE_1t/\hbar}\psi_1(x,0) + e^{-iE_2t/\hbar}\psi_2(x,0)\right)$$

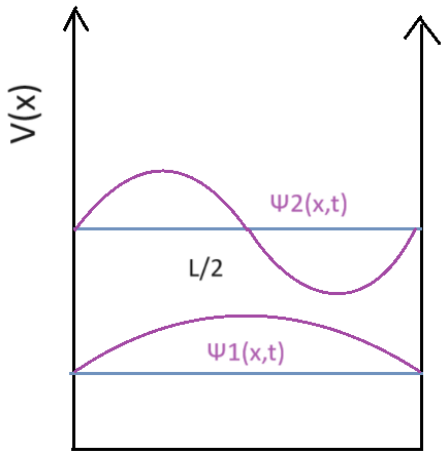
What do $|\psi_e(x,t)|^2$ and $|\psi_s(x,t)|^2$ look like? That is, do the maths and get expressions for $|\psi_e(x,t)|^2$ and $|\psi_s(x,t)|^2$. Why do these behave the way they do? Show this with drawings or screenshots from Composer!

Given for an eigenstate, $\psi_e(x,t) = e^{-iEt/\bar{h}}\psi(x,0)$

$|\psi_e(x,t)|^2 = \psi_e^*(x,t)\psi_e(x,t) = e^{iEt/\bar{h}}\psi^*(x,0)e^{-iEt/\bar{h}}\psi(x,0)$

$|\psi_e(x,t)|^2 = |\psi(x,0)|^2$

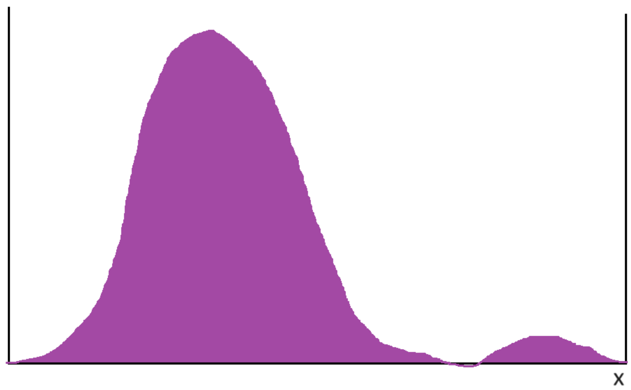
This shows $|\psi_e(x,t)|^2$ is independent of time. It behaves the way like this because this is the probability density, time should not affect.



Given for a superposition, $\psi_s(x,t) = \frac{1}{\sqrt{2}}(e^{-iE_1t/\bar{h}}\psi_1(x,0) + e^{-iE_2t/\bar{h}}\psi_2(x,0))$

$|\psi_s(x,t)|^2 = \frac{1}{2}|\psi_1(x)|^2 + \frac{1}{2}|\psi_2(x)|^2 + \frac{1}{2}(\psi_1^*(x)\psi_2(x)e^{-i(E_2-E_1)t/\bar{h}} + \psi_1(x)\psi_2^*(x)e^{i(E_2-E_1)t/\bar{h}})$

This shows $|\psi_s(x,t)|^2$ is time dependent. It behaves the way like this because superpositions evolve in time at different rates.

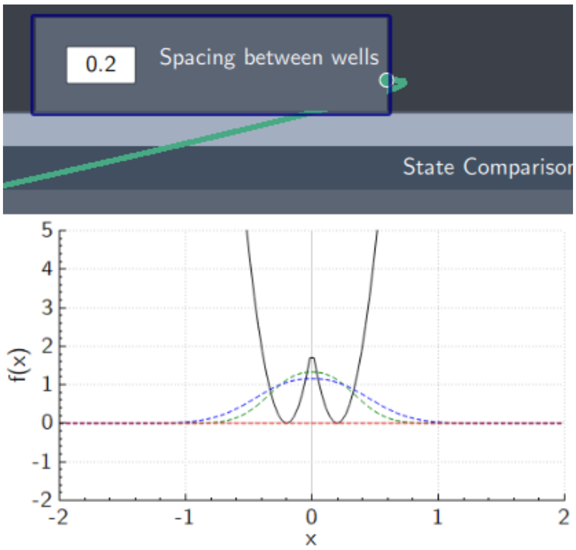


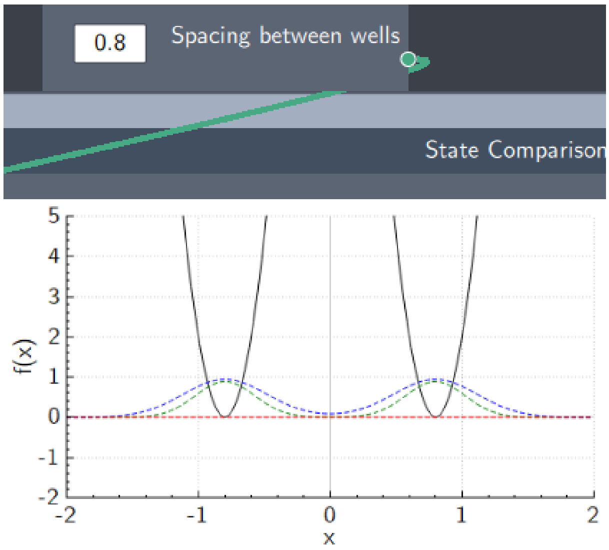
7. Open *double_well.flow*.

(i) Draw (or take screenshots of) the ground and the first excited state for this potential as you vary the separation between wells between 0 and 1.

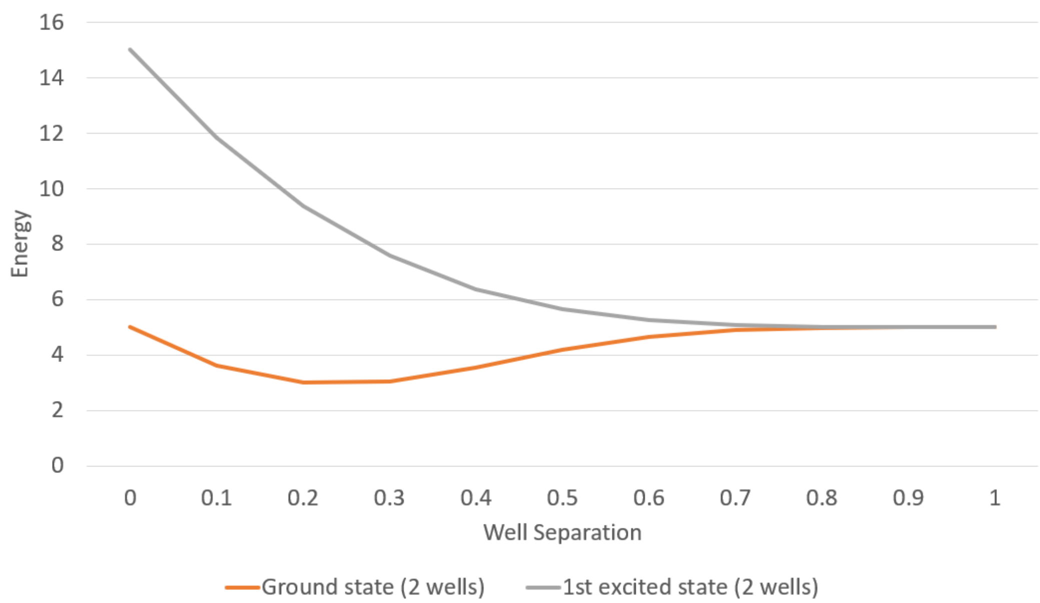
(ii) Plot the energies of the ground and first excited state for this two-well system. How do these vary as you change the well separation?

(i)





(ii)



Energy of ground state (2 wells) drops in the beginning as the well separation increases, and then increases as the well separation further increases, but at a certain point, the trend is very insignificant till the end.

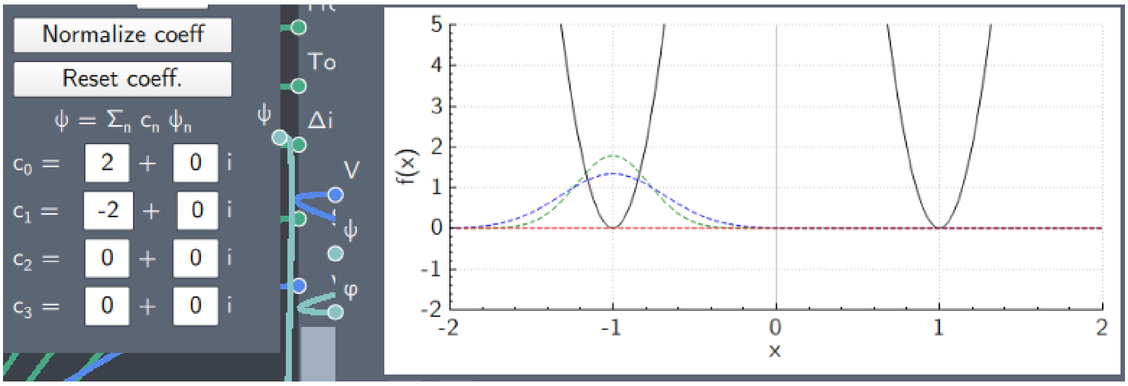
Energy of the 1st excited state (2 wells) significantly drops in the beginning as the well separation increases, and then slowly drops as the well separation further increases, but at a certain point, the trend is very insignificant till the end.

8. Now, using *double_well.flow*, try to vary the linear combination of c_0 and c_1 so that you make the following:

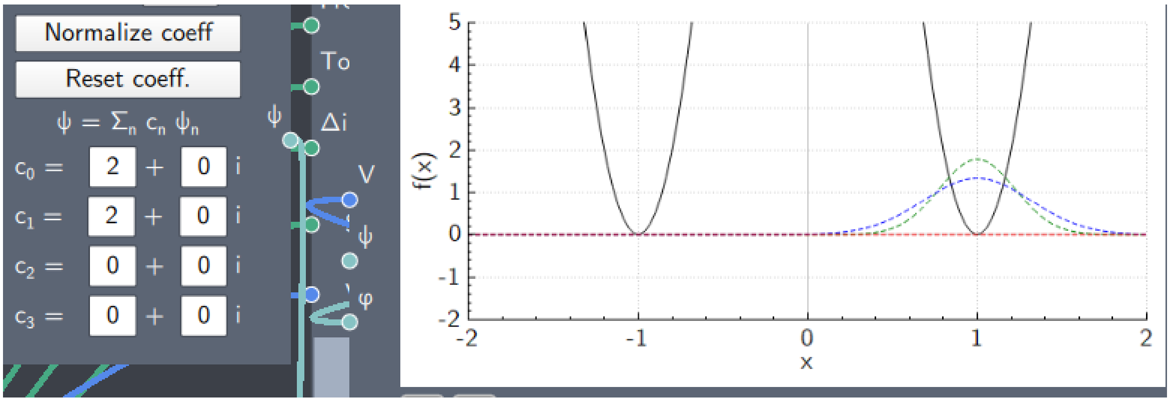
(i) A state localised to (i.e., located mostly in) the left well.

(ii) A state localised to the right well.

(i) Value of c0 and c1 has to be opposite to each other.



(ii) Value of c0 and c1 has to be the same to each other.



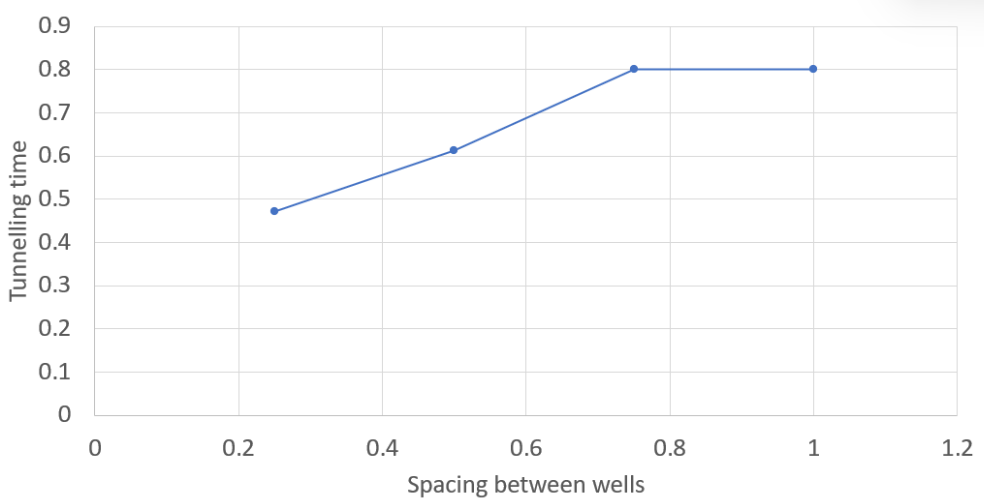
9. Study how the tunnelling rate varies as you change the spacing between wells between 0.25 and 1. Try to be as quantitative as you can! Let the system run for a total time and count how many oscillations you see as a function of the well spacing. The tunnelling time is then the number of oscillations divided by the total time you have run the system for. See the slides for this week's lecture for some images that show this.

(i) How does the tunnelling time change as you change the separation between wells? Plot this!

(ii) How does this compare to your plot of the energy separation vs. well spacing?

(iii) Explain: what is physically happening here? Can you describe this with maths?

(i) As the spacing between wells increases, the tunnelling time increases. The tunnelling time increases significantly in the beginning as we increase the spacing between wells, and then slowly increase as we further increase the spacing between wells.



(ii) To compare this with the energy vs well spacing plot, they share a similarity which both experience a significant trend in the beginning and a very insignificant trend at a certain point till the end.

(iii) To understand what is physically happening here, I need to understand how tunnelling happens first.

The Heisenberg uncertainty principle explains a limit on how exactly a particle's position and momentum may be determined at the same time. This tells that while a solution might approach infinite if, for e.g. the calculation for its position was taken as a probability of 1, the other, i.e. its speed, would have to be infinite. However, there are no solutions with a probability of exactly zero (or one). Because of this, there is a non-zero possibility that a particular particle will exist on the other side of an intervening barrier, and these particles will manifest on the "other" side at a relative frequency that is proportionate to this probability. So, physically in tunnelling, the particles have some probability of penetrating through the barrier without sufficient energy and appear on the other side of the box. But under what conditions can particles penetrate?

When a particle reaches a barrier it cannot overcome, a particle's wave function changes from sinusoidal to exponentially diminishing in form. The solution for the Schrödinger equation in such a medium is:

$\psi = Ne^{-\beta x}$,

where N is a normalisation constant and $\beta = \sqrt{\frac{2m(V-E)}{\bar{h}^2}}$

Three requirements need to be satisfied for a quantum particle in order to penetrate a barrier:

1. The barrier's thickness should be small and its height must be limited.
2. Particle’s kinetic energy < barrier’s potential energy (E < V).
3. Particles have wave characteristics.

Then, there would be a chance of finding the particles on the other side of the barrier if these requirements were satisfied. A particle starts out as a sinusoidal wave, tunnels through the barrier, and then experiences exponential decay until it breaks through. And then smaller-amplitude sinusoidal waves out the opposite side of the barrier.

The Schrödinger Equation provides the probability, P, of a particle tunnelling the barrier. It can be expressed as follows:

$P = exp(\frac{-4a\pi}{h}\sqrt{2m(V - E)})with\ E < V\ where$

- V is potential barrier
- E is KE by particle
- a is thickness of barrier
- m is mass of particle
- h is Planck's constant

From this equation, we can see that the probability of tunnelling decreases with the increasing gap between the energy of the object and the energy of the barrier. Since the probability is low, the tunnelling time is high. Furthermore, as the P is defined as an exponential function, it can have a slow and insignificant decay in the end. This explains why the graph in the previous subquestion experiences an insignificant trend in the later stages.