Interactive simulations for the learning and teaching of quantum mechanics concepts

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www.st-andrews.ac.uk/~qmanim

www.st-andrews.ac.uk/~ak81/IOPSims

http://quantumphysics.iop.org

The Higher Education Academy

IOP Institute of Physics

University of St Andrews 600 YEARS

MPTL'18, 11-13 September, Madrid

The QuVis team

- Development of simulations and accompanying activites: Antje Kohnle
- Students involved in coding: Liam Atkinson, Inna Bozhinova, David Canning, Christopher Carroll, Aleksejs Fomins, Joe Llama, Gytis Kulaitis and Martynas Prokopas
- Final year project students: Cory Benfield, Callum Ferguson and Bruce Torrance
- Faculty involved in evaluation: Charles Baily, Donatella Cassettari, Margaret Douglass, Tom Edwards, Noah Finkelstein, Alastair Gillies, Georg Hähner, Christopher Hooley, Friedrich Koenig, Natalia Korolkova and Bruce Sinclair

http://arxiv.org/abs/1307.1483
http://arxiv.org/abs/1307.1484

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Eur. J. Phys. 31 (2010) 1441-1455

Project motivation

- Simulations can enhance engagement, exploration of relationships between quantities and model-building through high levels of interactivity, prompt feedback, implicit scaffolding and multiple representations of concepts. [Singh, Belloni, and Christian 2006, Podolefksy et al 2010, McKagan et al 2008, Clark and Mayer 2011, Zollmann et al 2002 etc.]
- Simulations may be particularly useful for the teaching and learning of quantum mechanics.
  - Counterintuitive nature of quantum mechanics.
  - Abstract , far-removed from everyday experience.
  - Simulations can help build conceptual understanding independent of mathematical proficiency.

The QuVis collections

Simulations for physics students (50 simulations, introductory to advanced undergraduate level)

www.st-andrews.ac.uk/~qmanim

Simulations for chemistry students studying introductory quantum mechanics (18 simulations, tailored explanations and activities)

www.st-andrews.ac.uk/~qmanim/chemistry

Simulations for the Institute of Physics new introductory quantum mechanics curriculum (17 simulations so far)
www.st-andrews.ac.uk/~ak81/IOPSims

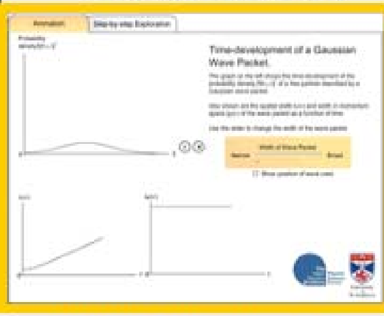
quantumphysics.iop.org

soon: all available at www.st-andrews.ac.uk/physics/quvis

QuVis: The University of St Andrews Quantum Mechanics Visualisation project

School of Physics & Astronomy

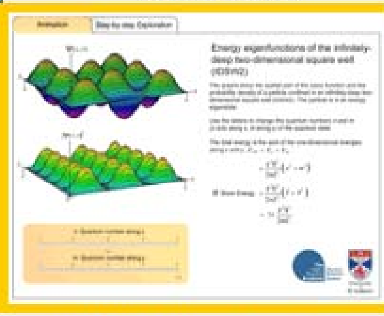
1 Gaussian Wave Packet



Problem Sets: pdf docx

Instructor resources: pdf docx

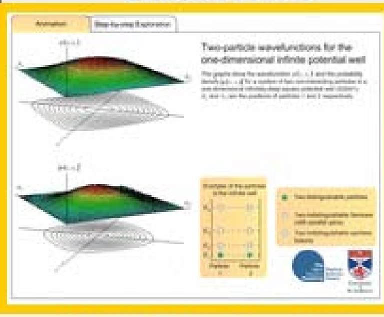
2 2D Infinite Well



Problem Sets: pdf docx

Instructor resources: pdf docx

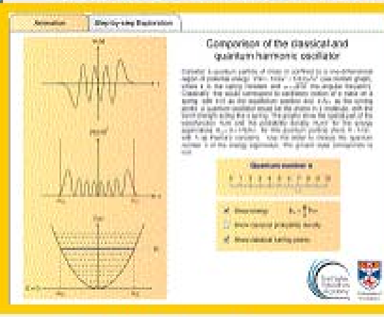
3 Fermions Bosons



Problem Sets: pdf docx

Instructor resources: pdf docx

4 1D Simple Harmonic Oscillator

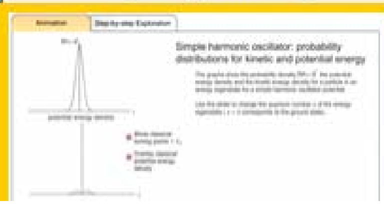


Problem Sets: pdf docx

Instructor resources: pdf docx

5 Momentum Probability Density

6 Energy Densities



QUANTUM PHYSICS

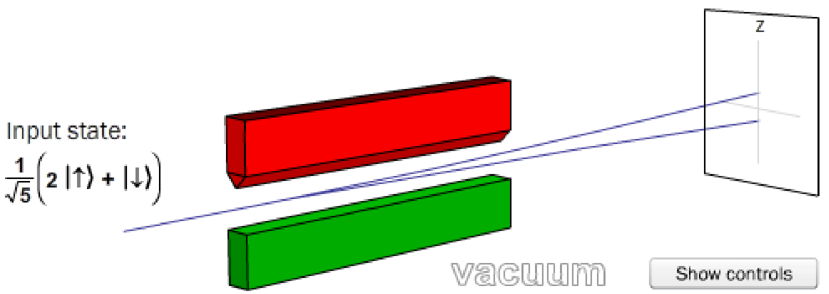
ANTJE

$$\hat{s}_z = \frac{1}{2}\hbar|\uparrow\rangle\langle\uparrow| - \frac{1}{2}\hbar|\downarrow\rangle\langle\downarrow| \,. \qquad (5)$$

In general, an observable quantity O in quantum mechanics is represented by an operator $\hat{o}$, and the average value obtained by repeated measurements of O on the state $|\psi\rangle$ is given by the expectation value $\langle O\rangle = \langle\psi|\hat{o}|\psi\rangle$.

Simulation | **Step-by-step Exploration** | quantumphysics.iop.org | University of St Andrews | IOP Institute of Physics

The expectation value of an operator



Consider a collimated stream of spin 1/2 particles. The particles pass through a Stern-Gerlach apparatus (SGA), which consists of a region of non-uniform magnetic field aligned along a given axis, here the z-axis. The SGA allows a measurement of the spin angular momentum component along this axis. For spin 1/2 particles, the particles separate into two discrete streams, one with spin component $S_z = +\frac{\hbar}{2}$ (here, deflection upwards), the other with spin component $S_z = -\frac{\hbar}{2}$ (here, deflection downwards). The spin 1/2 particles have all been prepared in the initial state $\frac{1}{\sqrt{5}}(2|\uparrow\rangle+|\downarrow\rangle)$, where $|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigenstates corresponding to $S_z = +\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ respectively.

Press the Show controls button to send particles through the SGA and to display various quantities.

FOUNDATIONAL

HISTORICAL

INFORMATIONAL

ARTICLES

Simulation activities

- Accompanying activities aim to promote guided exploration and sense-making, help students compare and contrast classical and quantum situations, and interpret their calculations with the experimental situations and data shown in the simulations.
- Solutions to all activities available to instructors (email ak81@st-andrews.ac.uk, for New Quantum Curriculum simulations quantumphysics@iop.org)
- Instructors are welcome to modify activities

"Explain how you can see these results graphically in the simulation".

"Using the simulation, come up with a general rule... ",

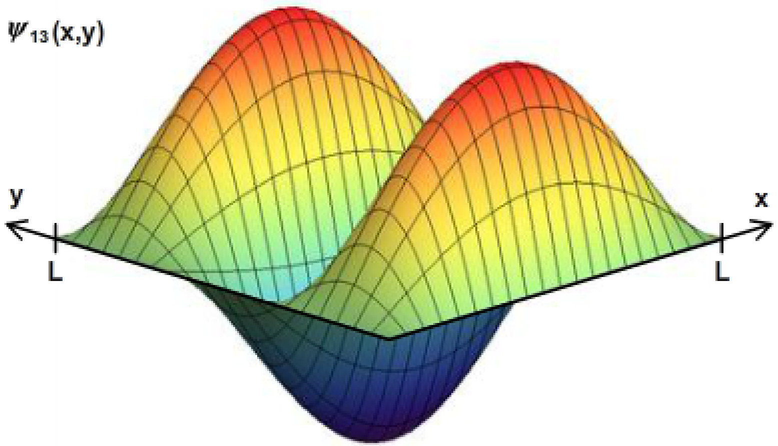
The IOP New Quantum curriculum

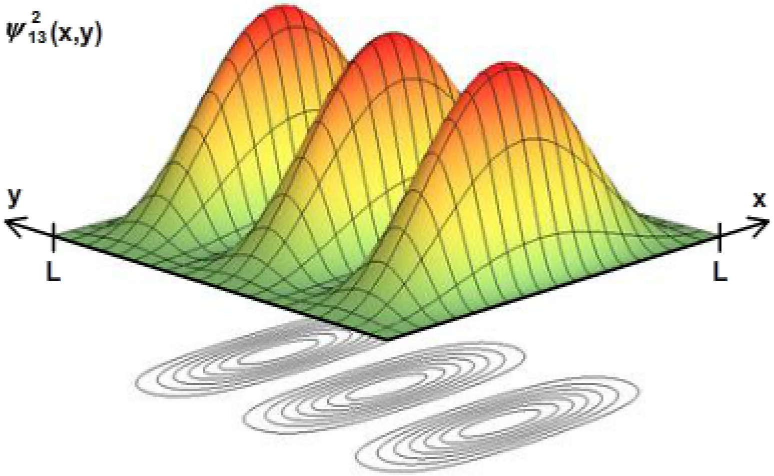
Review of approaches in the UK, IOP accredits all UK physics programmes.

Freely available online resources for a first university course in quantum physics developing the theory using two-level systems (single photon interference, spin ½ particles).

- Focus on experiments that have no classical explanation, interpretive aspects of quantum mechanics and quantum information theory
- Mathematically less challenging (much of the linear algebra needed part of the resource)

Animation | Step-by-step Exploration

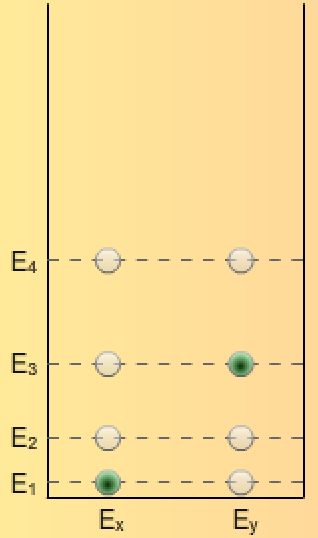




Comparison of one particle in a two-dimensional well and two particles in a one-dimensional well

The graphs show the first few wavefunctions and probability distributions for either one particle in a two-dimensional (2D) infinitely deep well or two distinguishable particles in a one-dimensional (1D) infinitely deep well. Use the buttons to choose the energies along x and y (for the one-particle case) or the energies of the individual particles (for the two-particle case).

Energies



Energies of the particle along x and y

Main controls

- One particle in a 2D square well
- Two distinguishable particles in a 1D well
- One particle in a 2D rectangular well

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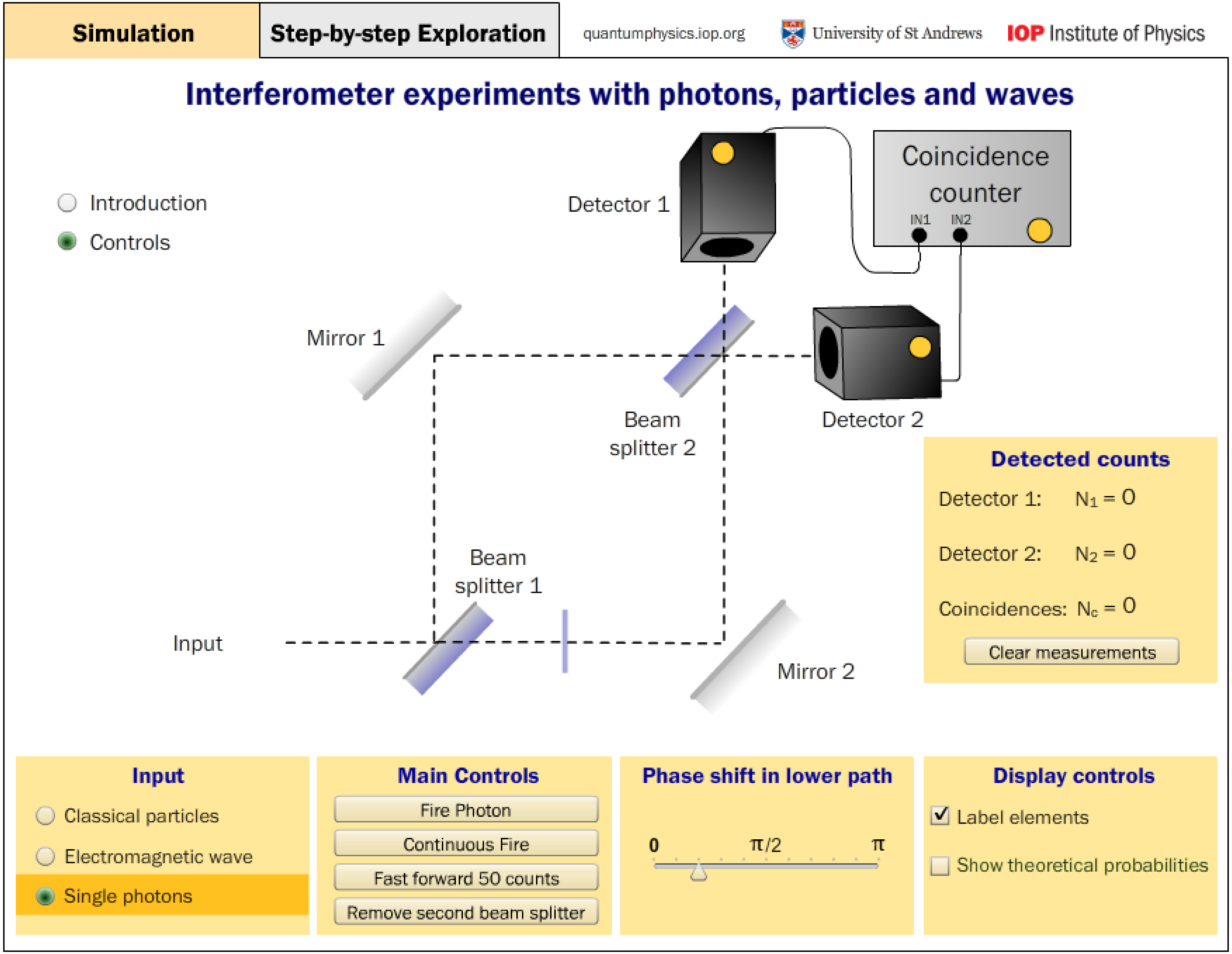

Simulation
Step-by-step Exploration
quantumphysics.iop.org
University of St Andrews
IOP Institute of Physics
Interferometer experiments with photons, particles and waves
Introduction
Controls
Detector 1
Coincidence counter
IN1
IN2
Mirror 1
Beam splitter 2
Detector 2
Detected counts
Detector 1: N1 = 0
Detector 2: N2 = 0
Coincidences: Nc = 0
Clear measurements
Beam splitter 1
Input
Mirror 2
Input
Classical particles
Electromagnetic wave
Single photons
Main Controls
Fire Photon
Continuous Fire
Fast forward 50 counts
Remove second beam splitter
Phase shift in lower path
0
π/2
π
Display controls
Label elements
Show theoretical probabilities

Simulation | Step-by-step Exploration

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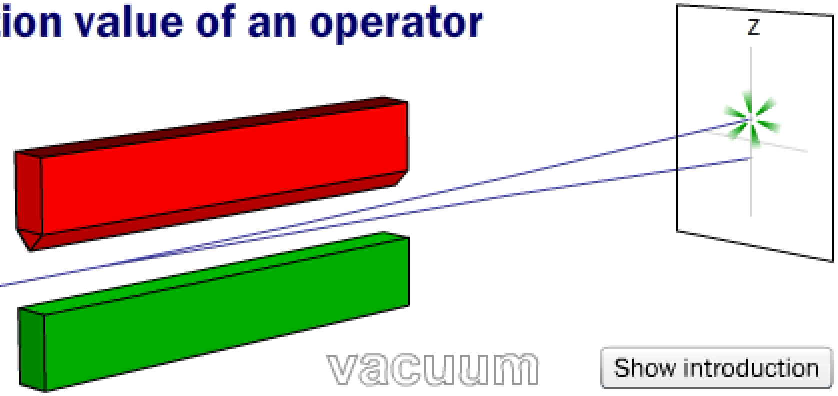
The expectation value of an operator

Input state:

- (selected) $\frac{1}{\sqrt{5}}\left(2\,|\uparrow\rangle + |\downarrow\rangle\right)$
- $a\,|\uparrow\rangle + b\,|\downarrow\rangle$ Find a and b!



Show introduction

Number of measurements

Total measurements: $N_{tot} = 56$

Outcome $S_z = +\frac{\hbar}{2}$: $N_+ = 50$

Outcome $S_z = -\frac{\hbar}{2}$: $N_- = 6$

Clear measurements

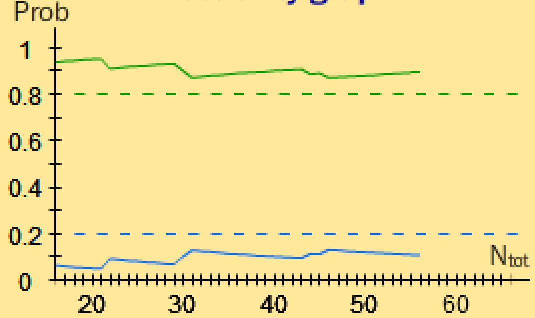
Main controls

Send spin 1/2 particles through the Stern-Gerlach apparatus

Take more measurements

- Single particle
- Continuous stream of particles
- Fast forward 50 particles

Probability graph



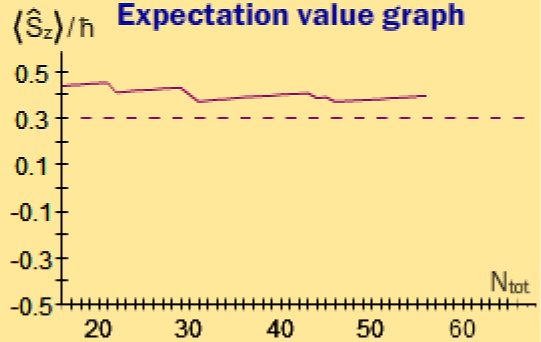
Probabilities

	Observed	Theoretical
$S_z = +\frac{\hbar}{2}$:	$Prob_+ = \frac{N_+}{N_{tot}} = 0.893$	0.8
$S_z = -\frac{\hbar}{2}$:	$Prob_- = \frac{N_-}{N_{tot}} = 0.107$	0.2

Display controls

- [x] Show probabilities
- [x] Show probability graph
- [x] Show expectation value
- [x] Show expectation value graph

Expectation value graph

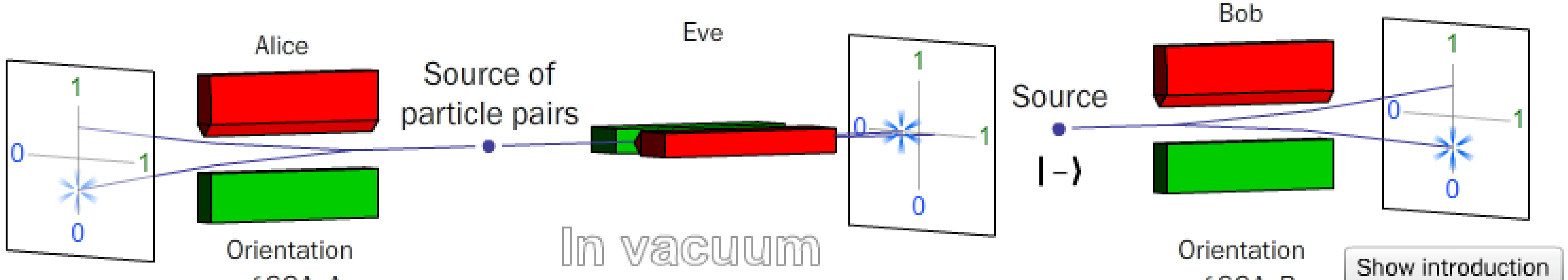


Expectation value

Mean of measurement outcomes	Theoretical
$\langle \hat{S}_z \rangle = (+\frac{\hbar}{2})Prob_+ + (-\frac{\hbar}{2})Prob_-$	
$\langle \hat{S}_z \rangle = 0.393\,\hbar$	$0.3\,\hbar$

Simulation | **Step-by-step Exploration** | quantumphysics.iop.org | University of St Andrews | IOP Institute of Physics

Quantum key distribution with entangled spin ½ particles



Show introduction

Z X — Random orientations — Fixed orientations — Z X

Main controls

Send entangled spin ½ particle pairs

Take more measurements

Single particle pair

Continuous stream of particle pairs

Fast forward 50 particle pairs

Let Eve intercept and resend particles

Stop eavesdropping

Alice		Eve		Bob		Alice and Bob	**Key**
Basis	Outcome	Basis	Outcome	Basis	Outcome	Same bases?	Bob inverts value
Z	0	X	0	Z	0	YES	ERROR
X	0	Z	1	X	0	YES	ERROR
X	0	Z	1	X	1	YES	0
X	1	X	0	Z	1	NO	
Z	1	Z	0	Z	0	YES	1
Z	0	Z	1	Z	1	YES	0
Z	0	Z	1	X	0	NO	

Display controls

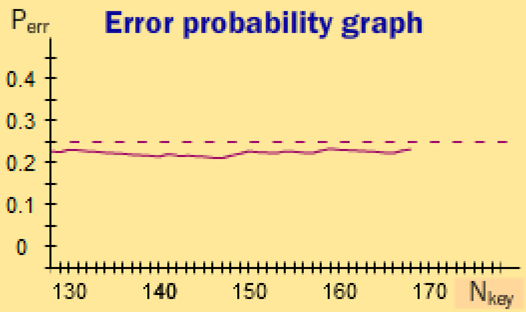
☑ Show secure key

☑ Show errors

☑ Show error probability graph

Clear measurements

Error probability graph



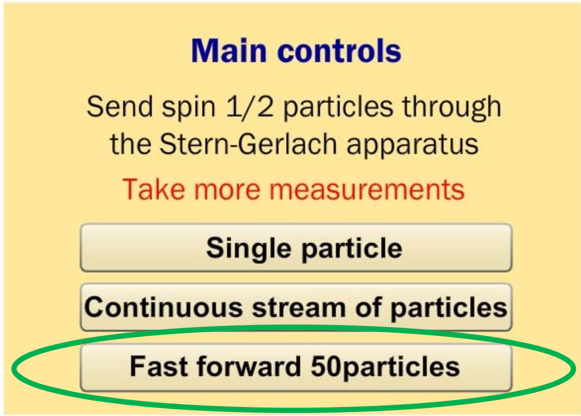
Errors

		Theoretical
Total pairs:	N_{tot} = 320	
Key bits:	N_{key} = 168	$0.5\,N_{tot}$
Errors:	N_{err} = 39	$0.25\,N_{key}$
Probability:	$P_{err} = \frac{N_{err}}{N_{key}} = 0.232$	0.25

Optimization of simulations and activities

- **Iterative refinement using student feedback essential for developing resources useful to students.**
- Example IOP simulations: 38 hours of observation sessions with 17 student volunteers in February/May 2013 from the St Andrews introductory level.
- Use of two simulations (single photon interference, hidden variables) in the Boulder modern physics course
- Use of three simulations (+ entanglement) in the St Andrews quantum physics course.
- Revisions to all simulations and activities where appropriate
- For other QuVis simulations: observation sessions in computer classrooms, conceptual diagnostic surveys

Example: Optimization of a simulation control



- In-class trials of two simulations in Boulder: 6 of 40 and 16 of 42 suggestions for improvement pertained to speeding up data collection.
- Added "Fast-forward" control prior to use at St Andrews. No suggestions for improvement (of 59) pertained to speed of data collection.
- Observation sessions: Controls typically explored top to bottom. Justifies layout. Student comments on usefulness of these controls.
- Control now incorporated into all simulations where data is collected.

Future activities

- Multi-institutional observation sessions and trials in introductory quantum courses with pre- and post-tests. Volunteers very welcome!
- Build a community of users (instructor resources, exemplars of use, user forum).
- Further simulations (+ all as HTML5/JS touchscreen versions) and additional activities (more exploratory and collaborative in nature). First HTML5 sims available soon.
- Investigate student difficulties with the New Quantum Curriculum. Further develop simulations based on outcomes.