

# Upgrad QM (Course: 5020-21)

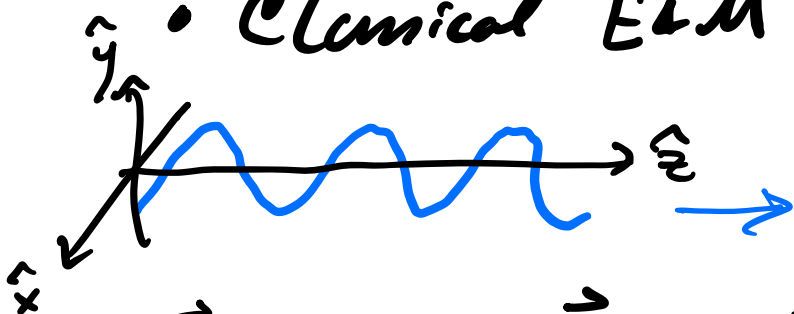
Braunstein 316, MWF 12:20-1:15

## Admin

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- [homepages.uc.edu/~angyrepc/](http://homepages.uc.edu/~angyrepc/)
- Townsend "Modern Intro QM" (2<sup>nd</sup> ed)
- 2<sup>nd</sup> course in QM!
- Broad outline:
  - F-semester: foundations
  - S-semester: basic applications & methods

## Motivation

- Classical E&M (light)



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

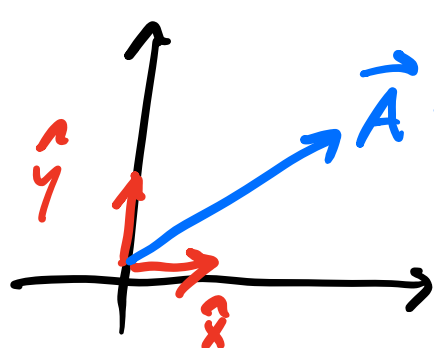
$$\vec{E} = A \hat{n} \cos(\vec{k} \cdot \vec{x} - \omega t + \theta)$$

amp.  $\uparrow$   $A \propto \sqrt{I}$   $\downarrow$  prob.  $\uparrow$  particles  
pol.  $\uparrow$   $\hat{n} \cdot \hat{k} = 0$   $\downarrow$  aug. mom. (spin/helicity)  
w. vect.  $\uparrow$   $\vec{k} = \text{div.}$   $\downarrow$  momentum  
freq.  $\uparrow$   $\omega = ck$   $\downarrow$  energy  
phase  $\uparrow$   $\omega = 2\pi\nu$   $\downarrow$  QM phase  
 $k = 2\pi/\lambda$

$$z = \text{Re} \left( A \hat{n} e^{i(\theta + \vec{k} \cdot \vec{x} - \omega t)} \right)$$

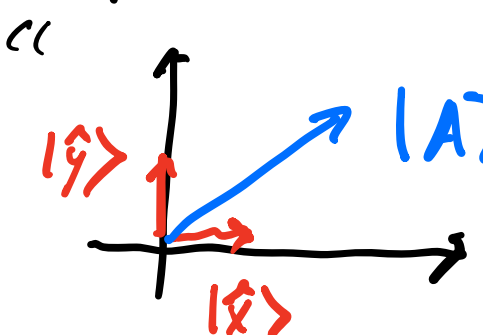
2d complex vector  $\rightarrow$  phase responsible for interference.  
"amplitude"

2d real vectors  $\vec{A}$



$$\vec{A} = A_x \hat{x} + A_y \hat{y} \sim \begin{pmatrix} A_x \\ A_y \end{pmatrix} \in \mathbb{R}$$

2d cplx vector:  $\vec{A} \rightarrow |A\rangle$  "ket"



$$|A\rangle = A_x |\hat{x}\rangle + A_y |\hat{y}\rangle \sim \begin{pmatrix} A_x \\ A_y \end{pmatrix} \in \mathbb{C}$$

transpose

$$\vec{A} = A \hat{n} \quad A = |\vec{A}| = \sqrt{\vec{A} \cdot \vec{A}} = \sqrt{\vec{A}^T \vec{A}}$$

$$= \sqrt{(A_x \ A_y) \begin{pmatrix} A_x \\ A_y \end{pmatrix}} \quad \text{"norm"} \geq 0$$

hermitian conj.  
"dagger"

$$\| |A\rangle \| = \sqrt{\langle A | A \rangle} = \sqrt{(|A\rangle^\dagger |A\rangle)}$$

"bra"

$$= \sqrt{(A_x^* \ A_y^*) \begin{pmatrix} A_x \\ A_y \end{pmatrix}} \geq 0$$

complex conj.

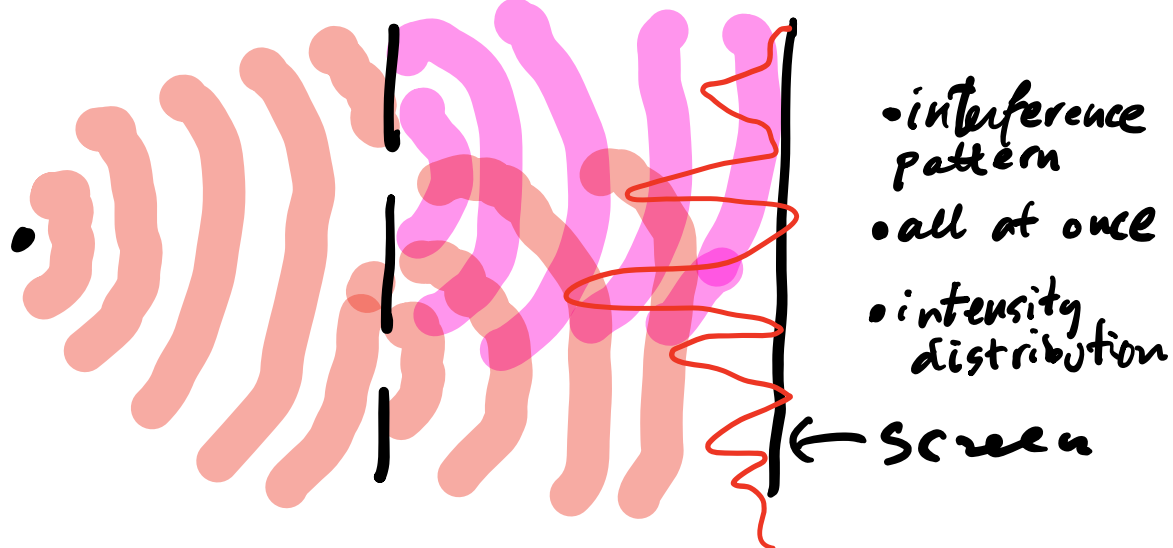
$$\vec{A} \cdot \vec{B} \in \mathbb{R} \quad \langle A | B \rangle \in \mathbb{C}$$

"bracket", "inner product".

Cplx vector space w inner product:  
"Hilbert space"

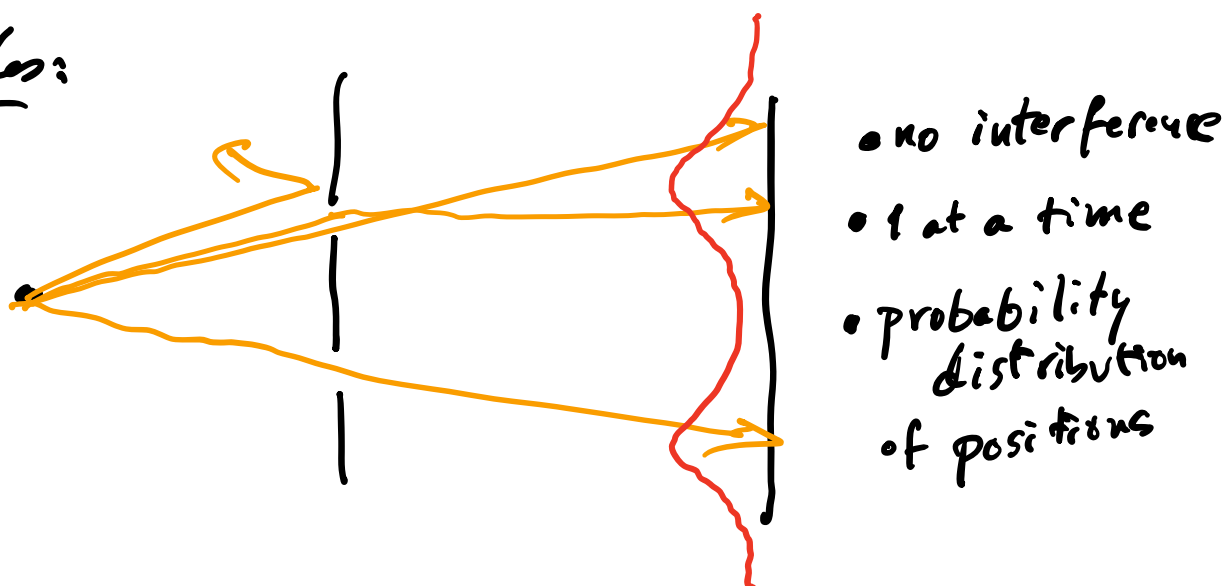
$$\langle A | \equiv |A\rangle^\dagger$$

Waves:



What happens as  $A \rightarrow 0$ ?

Particles:



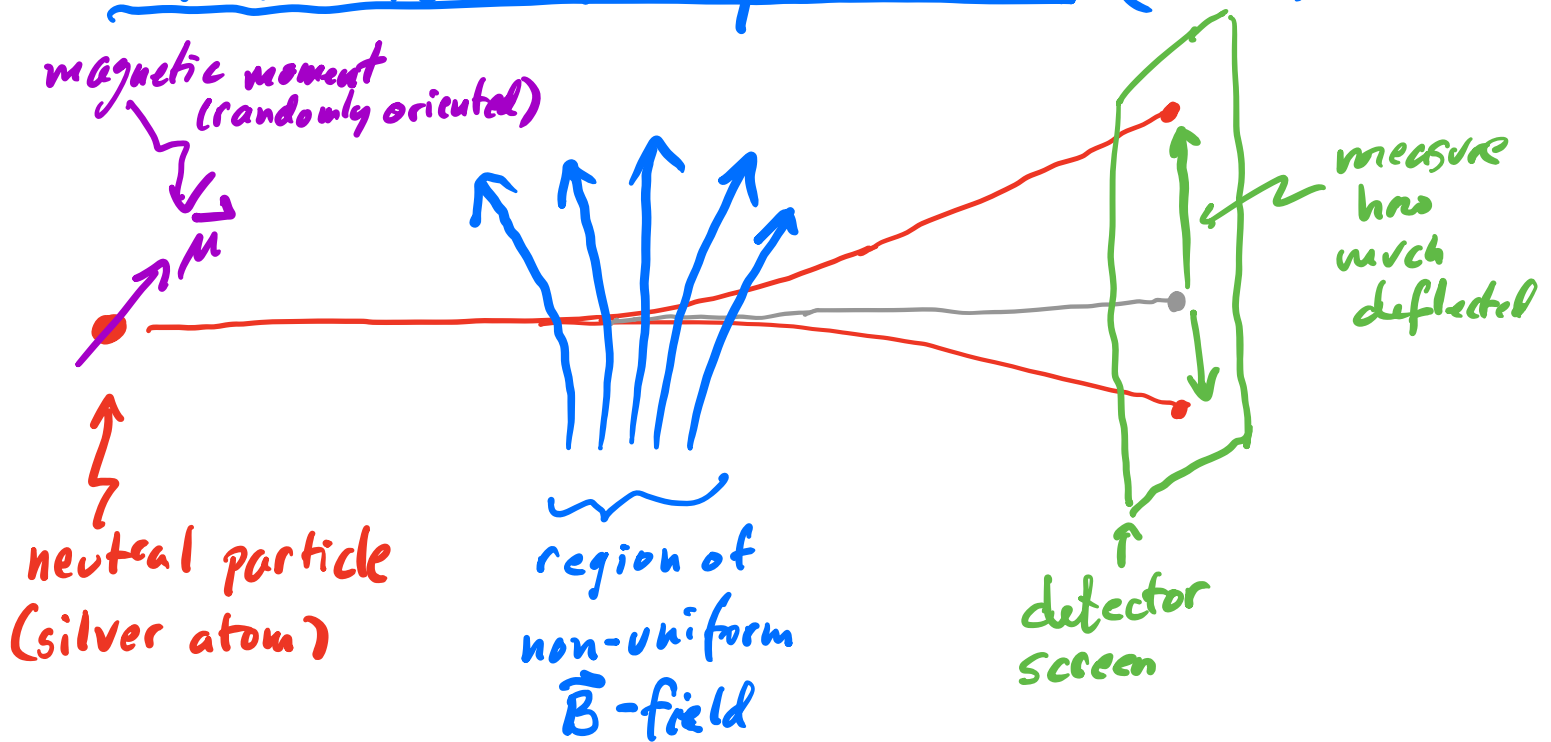
What happens when make holes v. small?

Experiment: same answer in both cases!

- light &  $e^-$ : both interfere
- " " : both give prob. dist. of individual "hits" on screen

History: (1900 Planck) & 1905 Einstein:  
light discrete  $E = n h \nu$   $n \in \mathbb{Z}$   
 $h \approx 6.626 \times 10^{-34} \text{ erg}\cdot\text{s}$

# Stern Gerlach experiments (ch. 1)



What do we expect classically?

- Energy of neutral particle in  $\vec{B}$ -field is  
$$V = -\vec{\mu} \cdot \vec{B}$$

$\Rightarrow$  Force is 
$$\vec{F} = -\vec{\nabla} V = \sum_{i=x,y,z} \mu_i (\vec{\nabla} B_i)$$

- Arrange  $\vec{B}$ -field so that

$$\vec{\nabla} B_z \approx \hat{e}_z \frac{\partial B_z}{\partial z} \quad \& \quad \text{rest } \vec{\nabla} B_i \approx 0$$

$$\Rightarrow \vec{F} = \hat{e}_z \mu_z \frac{\partial B_z}{\partial z}, \quad \text{so:}$$

displacement in  $z$ -direction,  $\propto \mu_z$ .



$$\bullet \vec{\mu} = \frac{q\hbar}{2mc} \vec{S}$$

w/

- $q$  = charge of particle (e.g.  $q = -e$  for  $e^-$ )
- $m$  = mass "
- $c$  = speed of light
- $g/2$  = numerical fudge factor ( $g \approx 2.0011...$  for  $e^-$ )
- $\vec{S}$  = angular momentum of particle
- = a.k.a. "spin"

We divide angular momentum into  
"spin" & "orbital" parts

$\vec{S}$  = spin = ang. mom. of particle coming from spinning on an axis through its center

$\vec{L}$  = orbital = ang. mom. of particle coming from its motion relative to the origin

$$\vec{J} = \text{Total ang. mom.} = \sum_{a=\text{particle}} (\vec{S}_a + \vec{L}_a) \quad \left\{ \begin{array}{l} \text{sum contributions} \\ \text{from all particles} \\ \text{making up atom} \end{array} \right.$$

- Silver atom: particles = 1 nucleus, 47  $e^-$ 's

$$\therefore \vec{J} = \vec{J}_N + \sum_{a=1}^{147} (\vec{S}_a + \vec{L}_a).$$

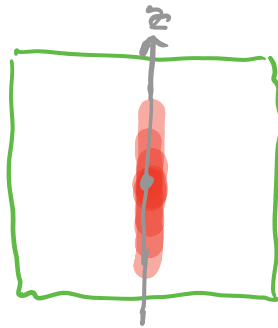
$$\therefore \vec{\mu}_{Ag} \sim \frac{g_N \cdot (47e)}{2m_N c} \vec{S}_N + \sum_{a=1}^{47} \frac{2(-e)}{2m_e c} (\underbrace{\vec{S}_a}_{\text{orange}} + \underbrace{\vec{L}_a}_{\text{green}})$$

$$\begin{array}{ccc}
 \underbrace{\quad}_{ss} & \frac{-e}{m_e c} \vec{S} & \underbrace{\quad}_{\uparrow\downarrow} \\
 (m_N \approx 2000 m_e) & (\text{all but one } e^- \text{ cancels}) & (\text{all cancel})
 \end{array}$$

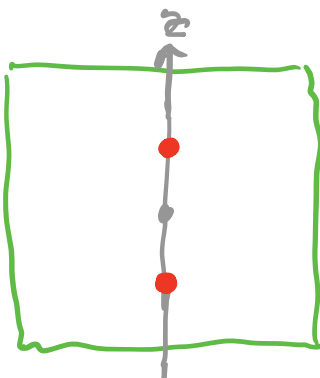
$$\Rightarrow \vec{\mu} \approx \frac{-e}{m_e c} \vec{S}_{\text{electron}}$$

$$\therefore \boxed{\mu_z \propto S_z} \quad \text{z-component of } e^- \text{ spin w/ computable coefficient}$$

$\Rightarrow$  Stern-Gerlach experiment should see a distribution of displacements of the silver atoms proportional to  $S_z$ , which is random.  
So expect to see on screen:



Instead, see:



Just two spots w/ equal probability

!!??  
...?

This makes no sense: even though the  $e^-$  spins were prepared completely randomly, their  $z$ -component takes just 2 specific values:

$$S_z = \begin{cases} +\hbar/2 & 50\% \text{ of time} \\ -\hbar/2 & 50\% \text{ of time} \end{cases}$$

$$[\hbar] = [\text{Energy} \times \text{Time}] = [\text{Mass} \times \text{Length}^2 / \text{Time}] = [\text{ang. mom.}]$$

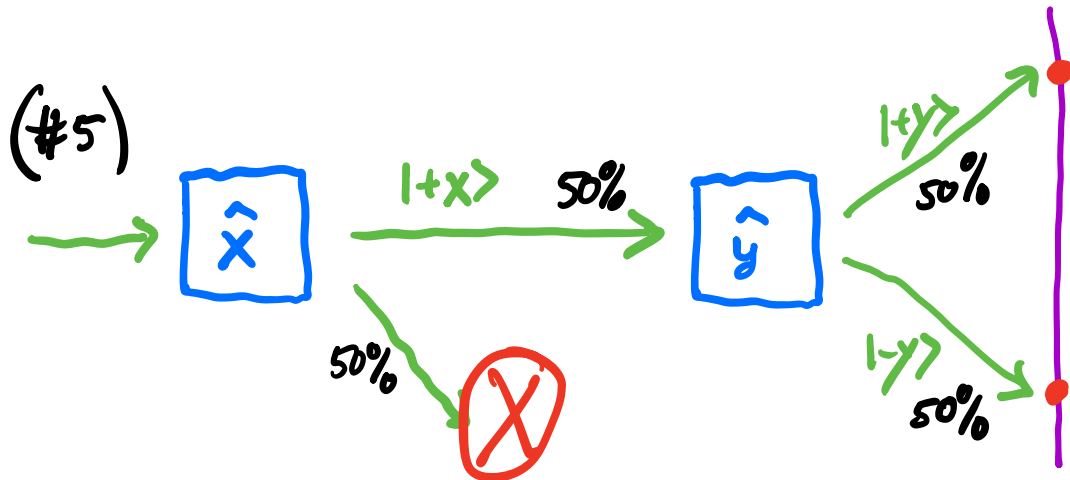
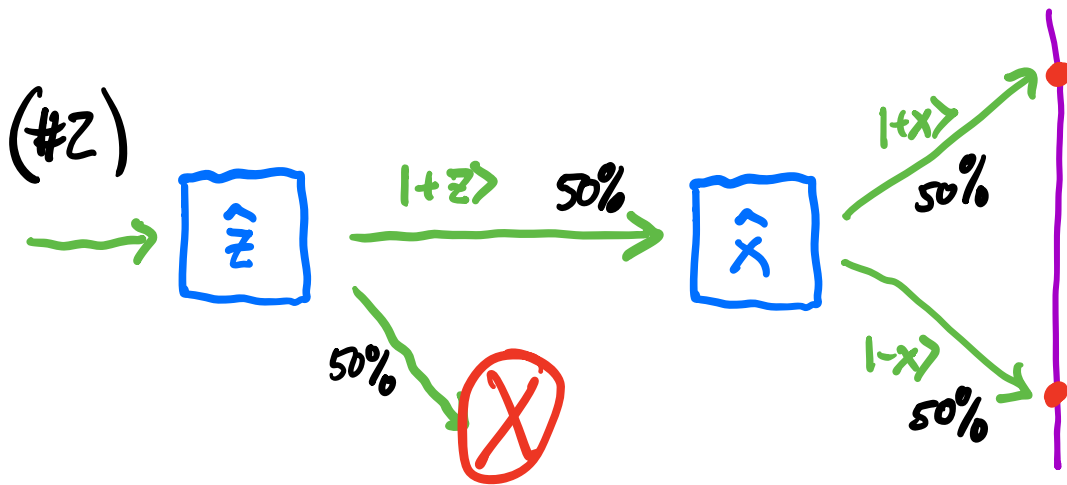
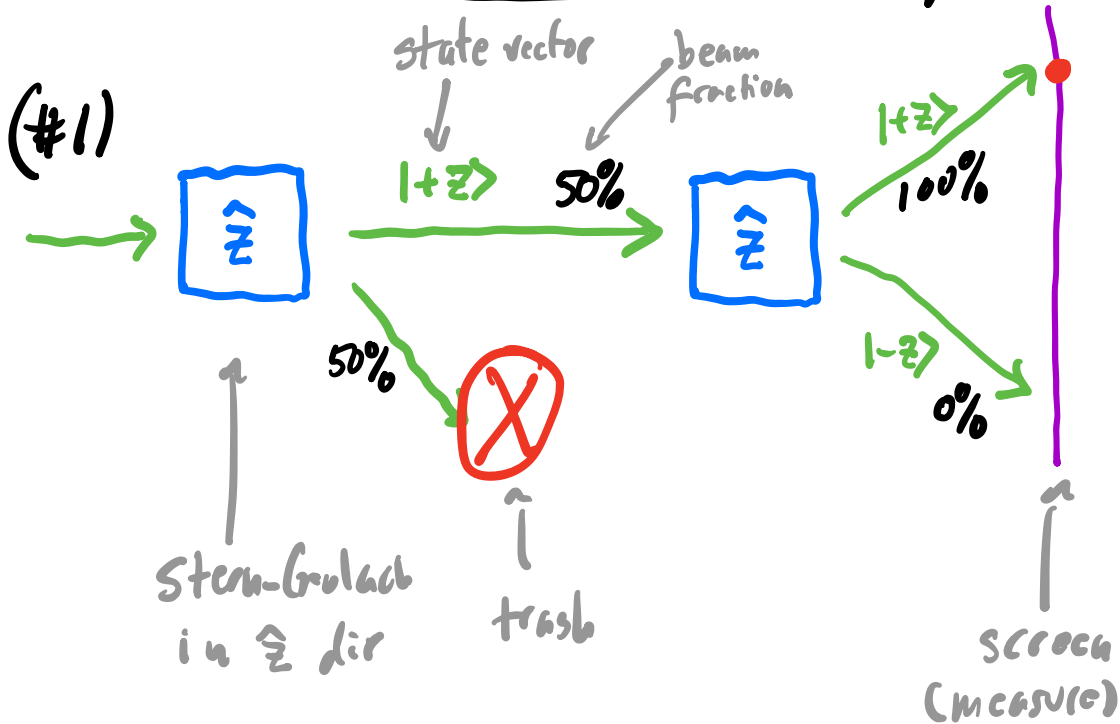
Will try to model this with vectors that add (to mimic wave interference).

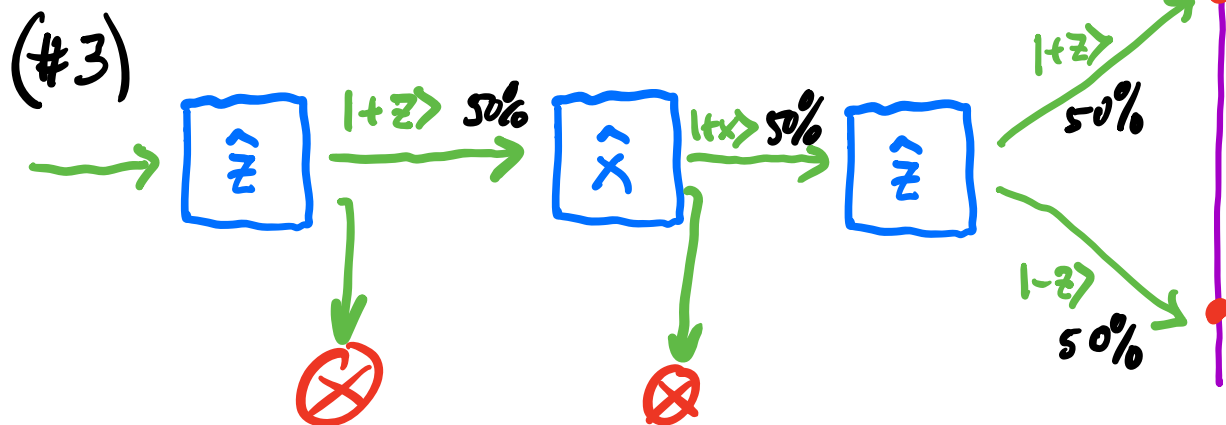
So define

$$|+\hat{z}\rangle \doteq \text{atom in state w/ } S_z = +\hbar/2$$

$$|-\hat{z}\rangle \doteq \text{ " " " " } S_z = -\hbar/2$$

## §1.2 some Stern-Gerlach experiments





§1.3) Given vector space rules of quantum mech.

- We motivated using vectors  $|+\hat{z}\rangle, |-\hat{z}\rangle$ , etc to describe spin states by analogy with polarization of waves.
- Intensity of wave  $\propto |\text{vector component}|^2$

E.g. intensity of part of wave  $\vec{A}$  polarized in  $\hat{n}$  direction is  $|\hat{n} \cdot \vec{A}|^2$

- Replace:  $\vec{A} \rightarrow |A\rangle$   
 Polariz.  $\hat{n} \rightarrow$  Stern-Gerlach outcomes  $|\pm \hat{n}\rangle$   
 $\vec{A} \cdot \vec{B} \rightarrow \langle A|B\rangle$

⇒ So guess rules for spins:

If send particles in spin state  $|\psi\rangle$  through a Stern-Gerlach magnet oriented in the  $\hat{n}$  direction, then there are **2 possible outcomes**:

- they come out in state  $|+\hat{n}\rangle$
- " " " " "  $|-\hat{n}\rangle$

(M)

with fractions (a.k.a. **probabilities**)

- $\text{Prob}(|\psi\rangle \Rightarrow |+\hat{n}\rangle) = |\langle +\hat{n} | \psi \rangle|^2$
- $\text{Prob}(|\psi\rangle \Rightarrow |-\hat{n}\rangle) = |\langle -\hat{n} | \psi \rangle|^2$

(B)

(M) = measurement rule: measurements have limited set of possible outcomes

(B) = Born rule: only probabilities of measurement outcomes are described.

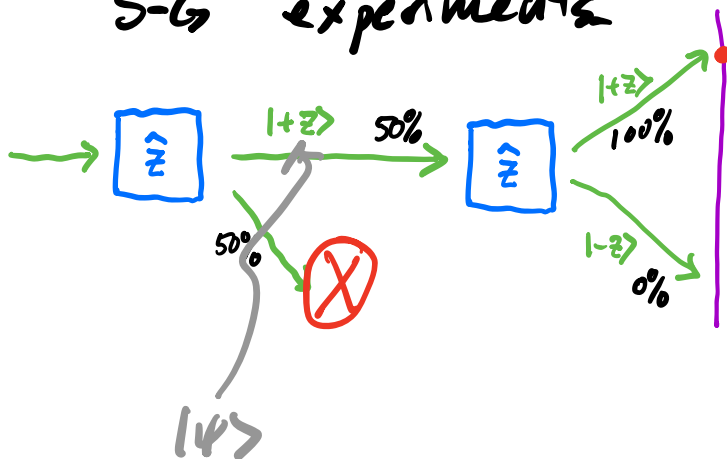
Use these rules, together with assumption that

$|\psi\rangle \in$  2-dimensional vector space ✓

(✓)

to model our S-G experiments

Experiment #1)



(B)  $\Rightarrow$

$$|\langle +z | \psi \rangle|^2 = |\langle +z | +z \rangle|^2 = 1 \Rightarrow \langle +z | +z \rangle = 1$$

$$|\langle -z | \psi \rangle|^2 = |\langle -z | +z \rangle|^2 = 0 \Rightarrow \langle -z | +z \rangle = 0$$

$$\text{Similarly w/ } |\psi\rangle = |-z\rangle \Rightarrow \langle -z | -z \rangle = 1$$

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

$\therefore \{ | +z \rangle, | -z \rangle \}$  forms an orthonormal basis of  $V$ .

$\Rightarrow$  any state  $|\psi\rangle$  can be written

$$|\psi\rangle = c_+ | +z \rangle + c_- | -z \rangle$$

$c_{\pm} \in \mathbb{C}$  are "components of  $|\psi\rangle$ " = "amplitudes"

$$\Rightarrow \langle +z | \psi \rangle = c_+ \langle +z | +z \rangle + c_- \langle +z | -z \rangle = c_+ \cdot 1 + c_- \cdot 0 = c_+$$

$$\therefore c_{\pm} = \langle \pm z | \psi \rangle \Rightarrow \text{Prob}(|\psi\rangle \Rightarrow |\pm z\rangle) = |c_{\pm}|^2$$

$\therefore$  (B)  $\Leftrightarrow$  "probabilities = |amplitudes|<sup>2</sup>"

$\Rightarrow$  probabilities  $\geq 0$  &  $\in \mathbb{R}$  ✓

Also want:  $\sum \text{probabilities} = 1$  ?

$$1 = \text{Prob}(|\psi\rangle \Rightarrow |+\rangle) + \text{Prob}(|\psi\rangle \Rightarrow |-\rangle) \\ = |c_+|^2 + |c_-|^2$$

$$\begin{aligned} \text{But } \langle \psi | \psi \rangle &= (c_+^* \langle +| + c_-^* \langle -|) (c_+ |+\rangle + c_- |-\rangle) \\ &= c_+^* c_+ \langle +|+\rangle + c_-^* c_+ \langle -|+\rangle \\ &\quad + c_+^* c_- \langle +|-\rangle + c_-^* c_- \langle -|-\rangle \\ &= |c_+|^2 \cdot 1 + c_-^* c_+ \cdot 0 + c_+^* c_- \cdot 0 + |c_-|^2 \cdot 1 \\ &= |c_+|^2 + |c_-|^2. \end{aligned}$$

$\therefore$  Physical states are normalized:

$$\boxed{\langle \psi | \psi \rangle = 1} \quad \textcircled{N}$$

Quantum weirdness: if both  $c_+ \neq 0$  &  $c_- \neq 0$ , then particle in state  $|\psi\rangle$  is not in state  $|+\rangle$  or  $|-\rangle$  but in a "superposition" of both.



Nevertheless, if measure  $|\psi\rangle$  using a Stern-Gerlach magnet in the  $\hat{z}$ -direction, get only 1 of 2 possible answers  $|+z\rangle$  or  $|-z\rangle$ .

$\therefore$  As a result of measurement, state changes

$$\left\{ \begin{array}{l} |\psi\rangle \Rightarrow |\psi'\rangle = |+z\rangle \\ \text{or} \\ |\psi\rangle \Rightarrow |\psi'\rangle = |-z\rangle \end{array} \right.$$



"collapse of w.v. fun."

## §1.4 & §1.5) Analysis of other SG experiments

These rules model other SG experiments consistently if:

$$\left\{ \begin{array}{l} |+x\rangle = \frac{1}{\sqrt{2}} (|+z\rangle + |-z\rangle) \\ |-x\rangle = \frac{1}{\sqrt{2}} (|+z\rangle - |-z\rangle) \end{array} \right.$$

and

$$\left\{ \begin{array}{l} |+y\rangle = \frac{1}{\sqrt{2}} (|+z\rangle + i|-z\rangle) \\ |-y\rangle = \frac{1}{\sqrt{2}} (|+z\rangle - i|-z\rangle) \end{array} \right.$$

this "i" is necessary & shows  $V$  must be a complex vector space

Check!  $\{| \pm x \rangle\}$  &  $\{| \pm y \rangle\}$  are also orthonormal bases of  $V$ .

## §1.6) Generalize our rules to "axioms of QM"

- (V) States are vectors  $|\psi\rangle \in V$  in a complex Hilbert space  $V$ .
- (N) States are normalized  $\langle\psi|\psi\rangle = 1$ .
- (M) The outcomes of a measurement "M" is an orthonormal basis of  $V$

$$\{|m_1\rangle, \dots, |m_k\rangle\} \quad \langle m_i | m_j \rangle = \delta_{ij}$$

Will call the  $|m_i\rangle$  an (orthonormal) "eigenbasis of M".

- (C) If an outcome  $|m_i\rangle$  is observed upon measuring  $M$ , then the state changes to

$$|\psi\rangle \xrightarrow{M=m_i} |\psi'\rangle = |m_i\rangle$$

- (B) The probability of observing an outcome  $|m_i\rangle$  of a measurement  $M$  is

$$\text{Prob}(|\psi\rangle \Rightarrow |m_i\rangle) = |\langle m_i | \psi \rangle|^2$$

- **Blue** = physical concepts  
**Purple** = math. concepts
  - Axioms essentially define a dictionary between **physics** and a **math. model**.
  - We will refine these axioms over the next few weeks to get to a (more) complete form.
  - The above axioms are missing any mention of **time evolution**; we have not given yet the quantum analog of the **equations of motion** ( $\vec{F} = m \ddot{\vec{x}}$ ).
- 

One subtle consequence of these rules is that the **overall phase** of a state is **physically unobservable**. i.e., no predictions of quantum mechanics depends on the overall phase.

Predictions are the probabilities computed by the Born rule **(B)**:

$$\text{Prob}(|\psi\rangle \Rightarrow |\chi\rangle) = |\langle \chi | \psi \rangle|^2$$

Say we have another state

$$|\psi'\rangle = e^{i\alpha} |\psi\rangle \quad \alpha \in \mathbb{R}$$

i.e., differing by an overall phase factor.  
Then

$$\begin{aligned} \text{Prob}(|\psi'\rangle \Rightarrow |\chi\rangle) &= |\langle \chi | \psi' \rangle|^2 \\ &= |\langle \chi | e^{i\alpha} |\psi\rangle|^2 \\ &= |e^{i\alpha} \langle \chi | \psi \rangle|^2 \\ &= |e^{i\alpha}|^2 |\langle \chi | \psi \rangle|^2 \\ &= |\langle \chi | \psi \rangle|^2 = \text{Prob}(|\psi\rangle \Rightarrow |\chi\rangle). \end{aligned}$$

So there is no way of telling the difference between  $|\psi'\rangle$  and  $|\psi\rangle$ .

(I used:  $|e^{i\alpha}|^2 = (e^{i\alpha})(e^{i\alpha})^* = e^{i\alpha} e^{-i\alpha} = e^{i\alpha - i\alpha} = e^0 = 1$ .)

Relative phases matter!

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

$$|\psi'\rangle = \frac{1}{\sqrt{2}} (|+\rangle + i|-\rangle)$$

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

$$i = e^{i\pi/2}$$

$$e^{i\alpha} = \cos\alpha + i\sin\alpha$$

Check:  
normalized!

$$\text{Prob}(|\psi\rangle \Rightarrow |\chi\rangle) = |\langle \chi | \psi \rangle|^2$$

$$= \left| \frac{1}{\sqrt{2}} (\langle +z | + \langle -z |) \frac{1}{\sqrt{2}} (|+z\rangle + |-z\rangle) \right|^2$$

$$= \left| \frac{1}{2} (\langle +z | +z \rangle + \langle +z | -z \rangle + \langle -z | +z \rangle + \langle -z | -z \rangle) \right|^2$$

$$= 1.$$

$$\text{Prob}(|\psi'\rangle \Rightarrow |\chi\rangle) = |\langle \chi | \psi' \rangle|^2$$

$$= \left| \frac{1}{\sqrt{2}} (\langle +z | + \langle -z |) \frac{1}{\sqrt{2}} (|+z\rangle + i |-z\rangle) \right|^2$$

$$= \left| \frac{1}{2} (\langle +z | +z \rangle + i \langle +z | -z \rangle + \langle -z | +z \rangle + i \langle -z | -z \rangle) \right|^2$$

$$= \left| \frac{1}{2} (1 + i) \right|^2 = \frac{1}{2} (1 + i) \frac{1}{2} (1 - i)$$

$$= \frac{1}{4} (1 + 1) = \frac{1}{2}.$$

# Expectation value and uncertainty

- When we do a measurement  $M$  on a system, we get a probability distribution of outcomes

$$P(|\psi\rangle \Rightarrow |m_i\rangle) = |\langle m_i | \psi \rangle|^2$$

$$\doteq P_i$$

← Shorthand notation

This just means that  $\{P_1, P_2, \dots, P_d\}$  are a set of  $d$  real numbers satisfying

$$0 \leq P_i \leq 1 \quad \& \quad \sum_{i=1}^d P_i = 1$$

- Say " $m_i$ " is the value of " $M$ " for the  $i$ -th outcome.

E.g. if  $M = S_z$ , then on a spin- $1/2$  system we have:

$$m_1 = -\hbar/2, \quad m_2 = +\hbar/2.$$

E.g. if  $M = E$  (energy), then on a hydrogen atom we have

$$m_n = - \frac{13.6 \text{ eV}}{n^2} \quad n = 1, 2, 3, \dots \infty$$

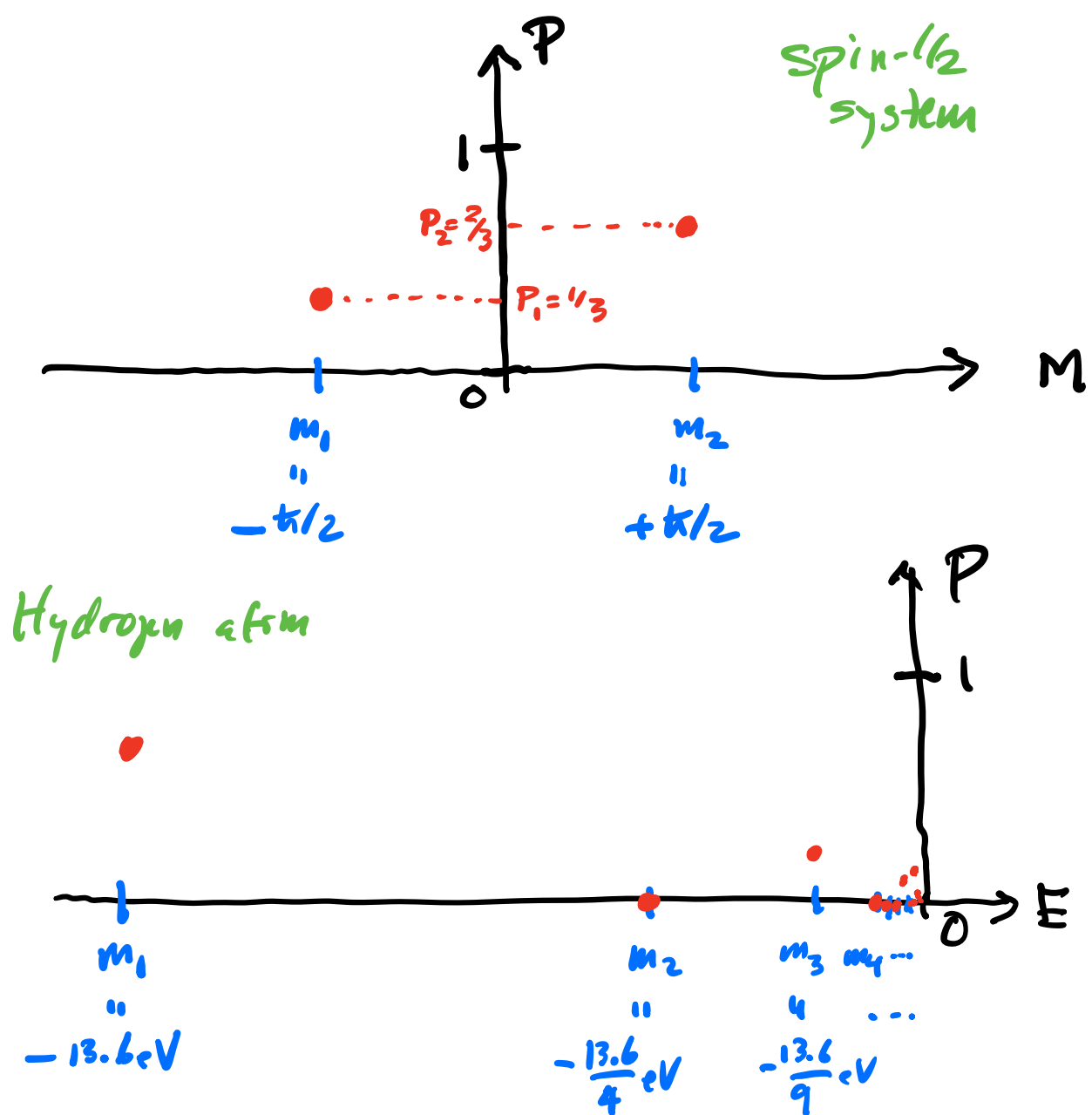
"electron volt"

- The numerical value of an outcome of a measurement " $m_i$ " and the probability of observing that outcome " $P_i$ " are completely different things!

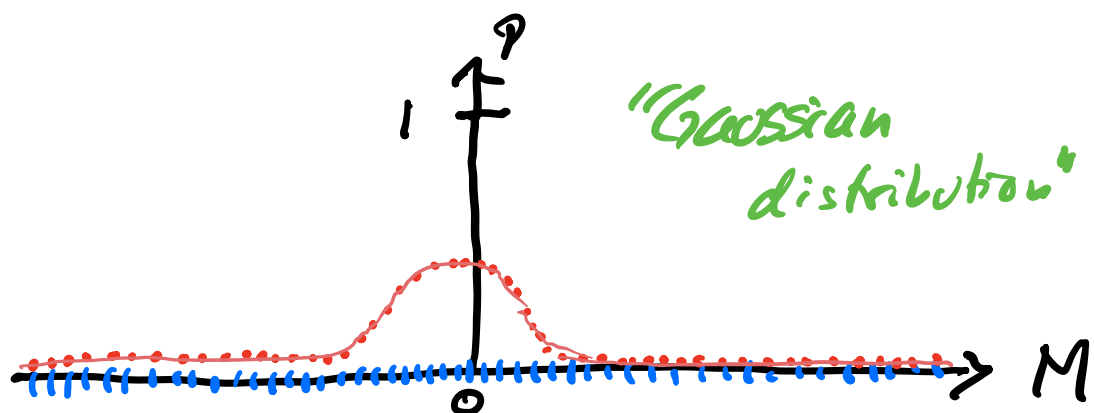
$\{m_i\}$  = property of the system,  
usually dimensionful quantities

$\{P_i\}$  = property of the state of the system,  
always a dimensionless number  
(between 0 & 1).

- Can visualize a probability distribution by plotting  $P_i$  vs.  $m_i$ :



- If the  $m_i$  are closely spaced, and  $P_i$  vary in small increments (i.e.  $|P_i - P_{i+1}| \ll 1$ ) can visualize as a continuous function





- Given a probability distribution two common questions are:

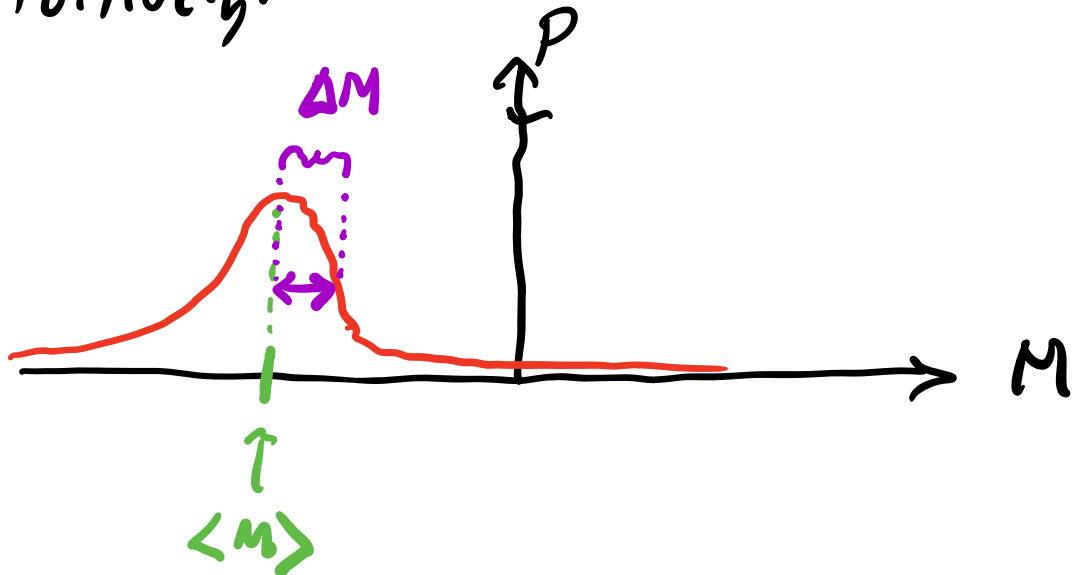
(1) What is the "average value" of  $M$   
 = "expected value" = "mean value"

$$\doteq \langle M \rangle \quad (= \langle M \rangle_{|\psi\rangle})$$

(2) What is the "uncertainty" of  $M$   
 = "standard deviation" = "width" = "variance"

$$\doteq \Delta M$$

Intuitively:



- Math definitions:

$$\langle M \rangle \doteq \sum_i m_i P_i = \sum_i m_i |\langle m_i | \psi \rangle|^2$$

$$\Rightarrow \langle f(M) \rangle \doteq \sum_i f(m_i) P_i \quad (\text{any function } f)$$

e.g.  $\langle M^2 \rangle \doteq \sum_i m_i^2 P_i$

$$\langle a f(M) \rangle = a \langle f(M) \rangle$$

↙ number

Note:

$$\langle f(M) + g(M) \rangle = \langle f(M) \rangle + \langle g(M) \rangle$$

$$\langle f(M) \cdot g(M) \rangle \neq \langle f(M) \rangle \cdot \langle g(M) \rangle$$

$$\Delta M \doteq \sqrt{\langle M^2 \rangle - \langle M \rangle^2}$$

Note:  $\Delta M \geq 0$ . Proof:

$$0 \leq \langle (M - \langle M \rangle)^2 \rangle = \langle M^2 - 2M\langle M \rangle + \langle M \rangle^2 \rangle$$

$$= \langle M^2 \rangle - \langle 2M\langle M \rangle \rangle + \langle \langle M \rangle^2 \rangle$$

$$= \langle M^2 \rangle - 2\langle M \rangle \langle M \rangle + \langle M \rangle^2 \cancel{\langle 1 \rangle}^1$$

$$= \langle M^2 \rangle - 2\langle M \rangle^2 + \langle M \rangle^2 = \langle M^2 \rangle - \langle M \rangle^2$$

$$= (\Delta M)^2$$

Exercise: justify every step!