

# INTRODUCTION TO DENSITY OPERATOR AND DENSITY MATRIX

Quantum Matter Theory's MBKM TEAM  
Research Center for Quantum Physics

Ref: Quantum Mechanics for Scientists and Engineers (David Miller, 2007)

# Pure and mixed states

So far the only randomness we have considered  
is from quantum-mechanical measurement

Consider, e.g., the state of polarization of a  
photon

So far, we could write a general state of  
polarization as

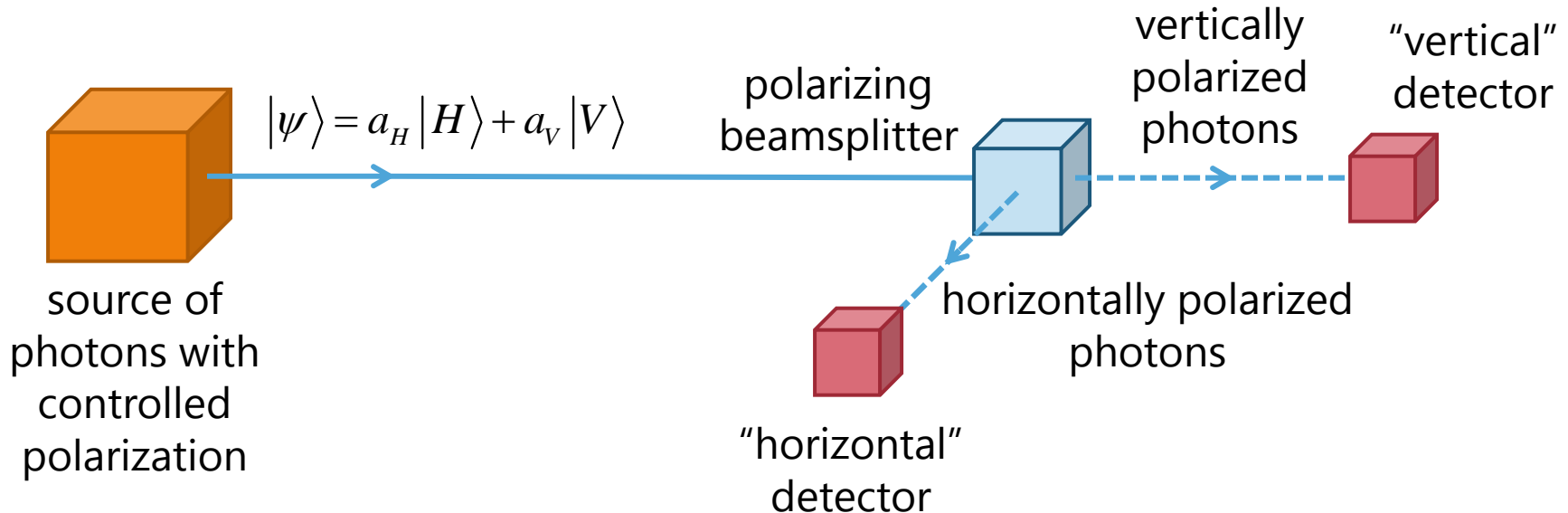
$$|\psi\rangle = a_H |H\rangle + a_V |V\rangle$$

where  $|H\rangle$  is a horizontally polarized  
photon state

and  $|V\rangle$  is a vertically polarized one

# Pure and mixed states

Suppose we measure such a state  $|\psi\rangle = a_H |H\rangle + a_V |V\rangle$   
using e.g., a polarizing beamsplitter that separates  
horizontal and vertical polarizations  
to different outputs with different detectors

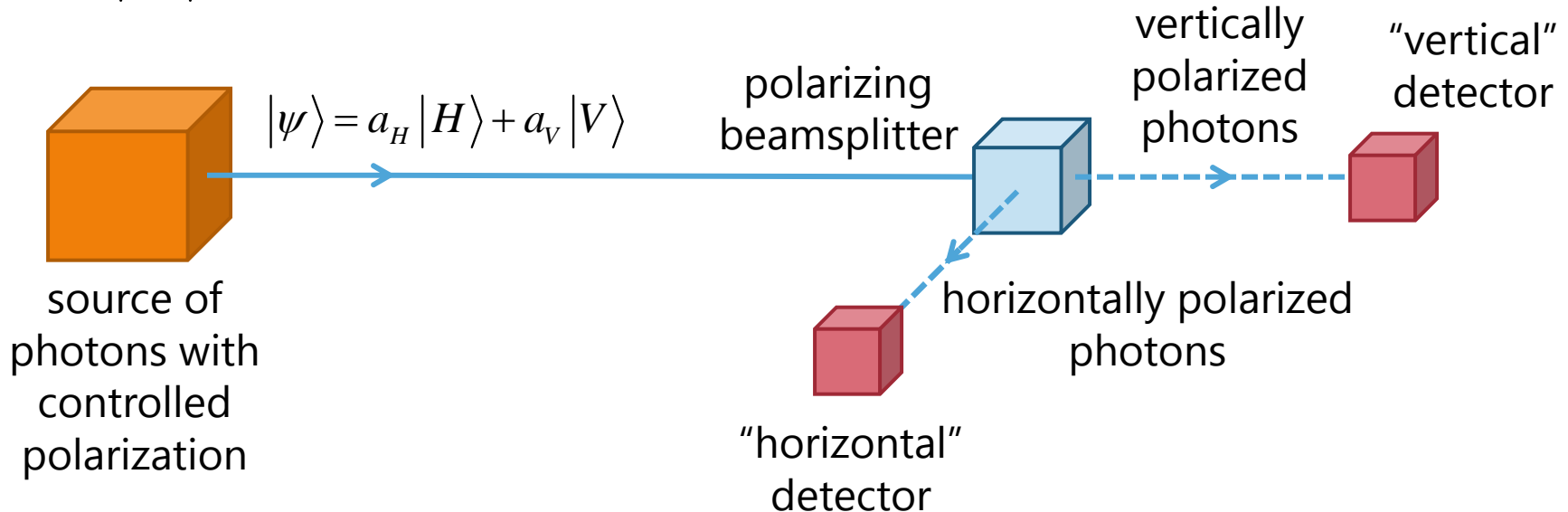


# Pure and mixed states

For this state,  $|\psi\rangle = a_H |H\rangle + a_V |V\rangle$  we expect probabilities

$|a_H|^2$  of measuring horizontal polarization

$|a_V|^2$  of measuring vertical polarization



## More complete description of optical polarization

Since we must have  $|a_H|^2 + |a_V|^2 = 1$  by normalization

we could also choose to write

$$a_H = \cos \theta \quad a_V = \exp(i\delta) \sin \theta$$

$\delta = 0$  corresponds to linear polarization

$\theta$  is then the angle of the optical electric vector  
relative to the horizontal axis

When  $\delta \neq 0$ , the field is in general “elliptically polarized”

the most general state of polarization

$\delta = \pm\pi/2$  with  $\theta = 45^\circ$  give

right and left circular polarization

# Polarization filter

We can always build a polarizing filter or compensator  
to allow passage of a photon of any specific polarization  
100% of the time

even when starting with elliptical polarization

We could arrange to delay only the horizontal polarization  
by a compensating amount  $-\delta$

to make the photon linearly polarized

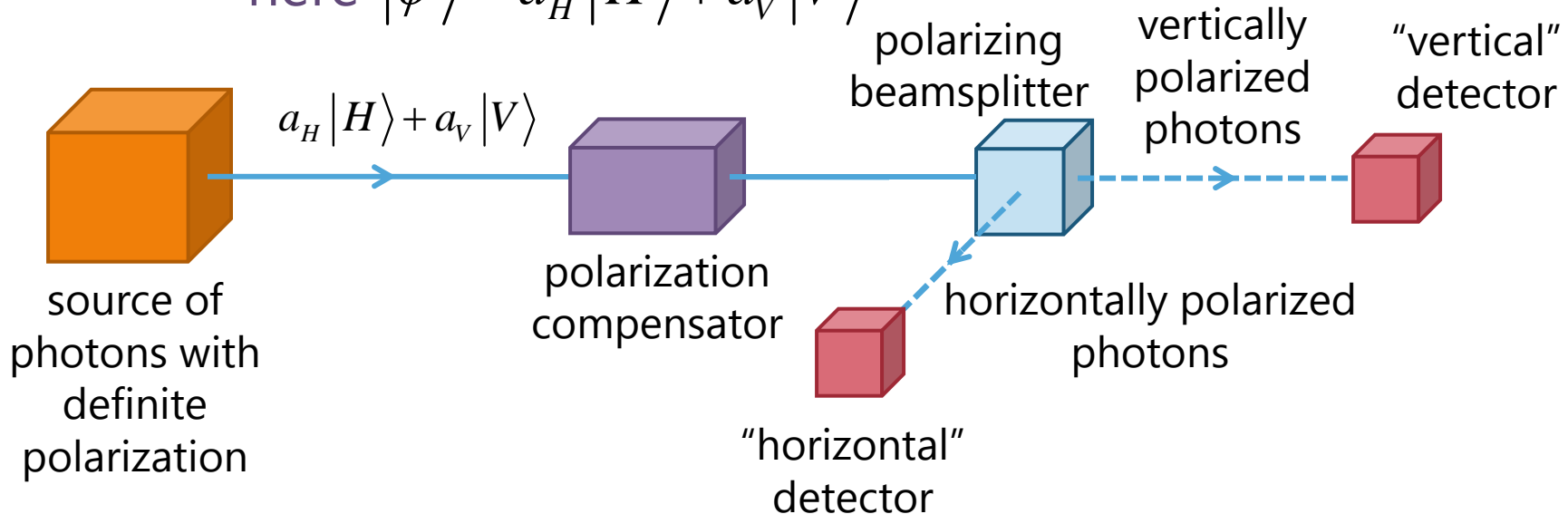
then rotate the polarization or apparatus by angle  $\theta$  so  
that the photon was always passed through

to, e.g., the vertical detector

# Pure states

When we can make a polarization filter or compensator  
so we get 100% of the photons to one detector  
we say that the photons are in a “pure” state

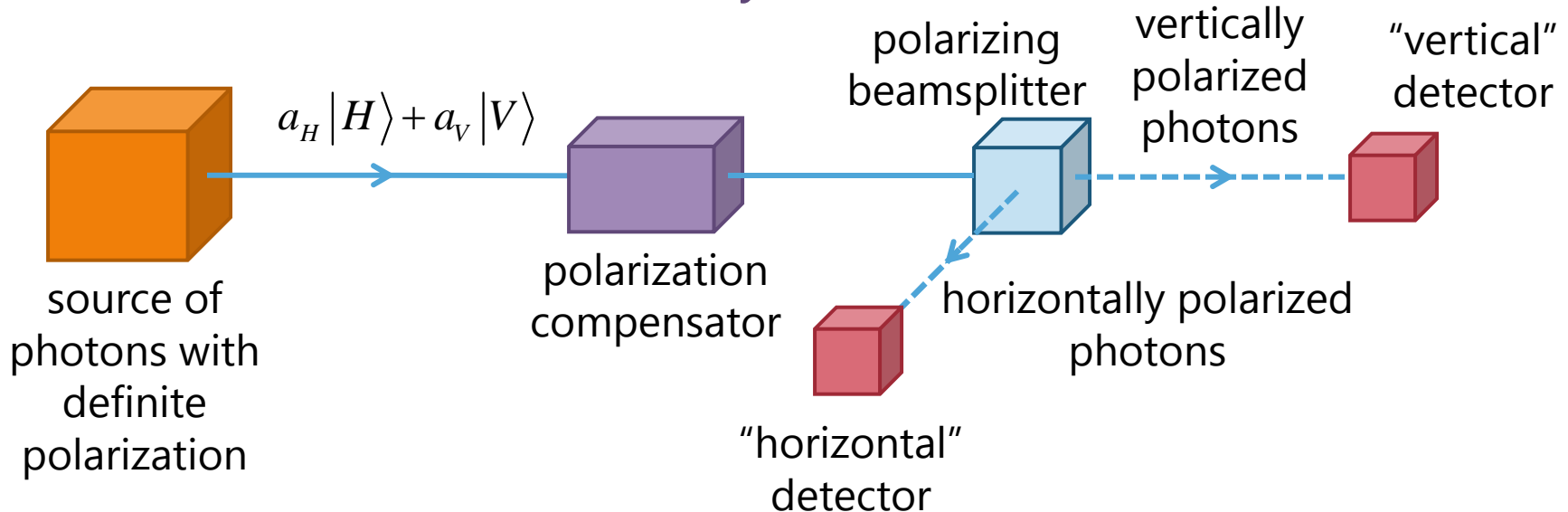
here  $|\psi\rangle = a_H |H\rangle + a_V |V\rangle$



# Pure states

All states considered so far have been pure states

A "compensator" could be made to pass any particles  
in any one specific quantum mechanical state  
with 100% efficiency to one detector





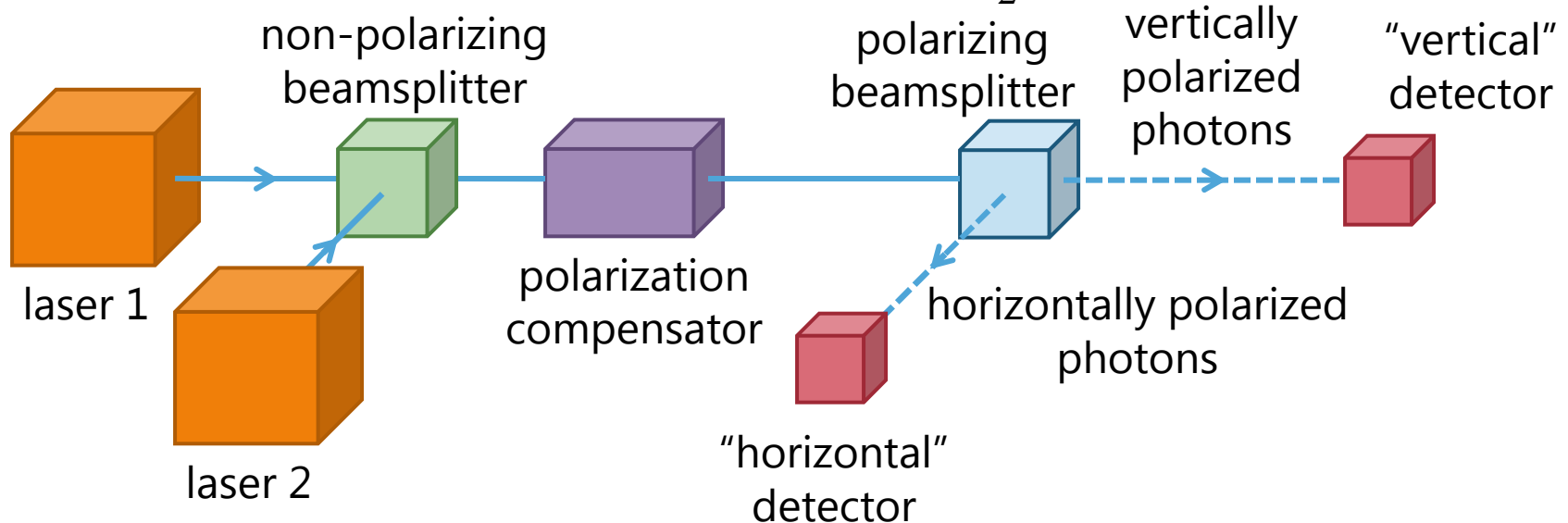
# Mixed states

Suppose we have a beam that is a mixture

from two different independent lasers, "1" and "2"

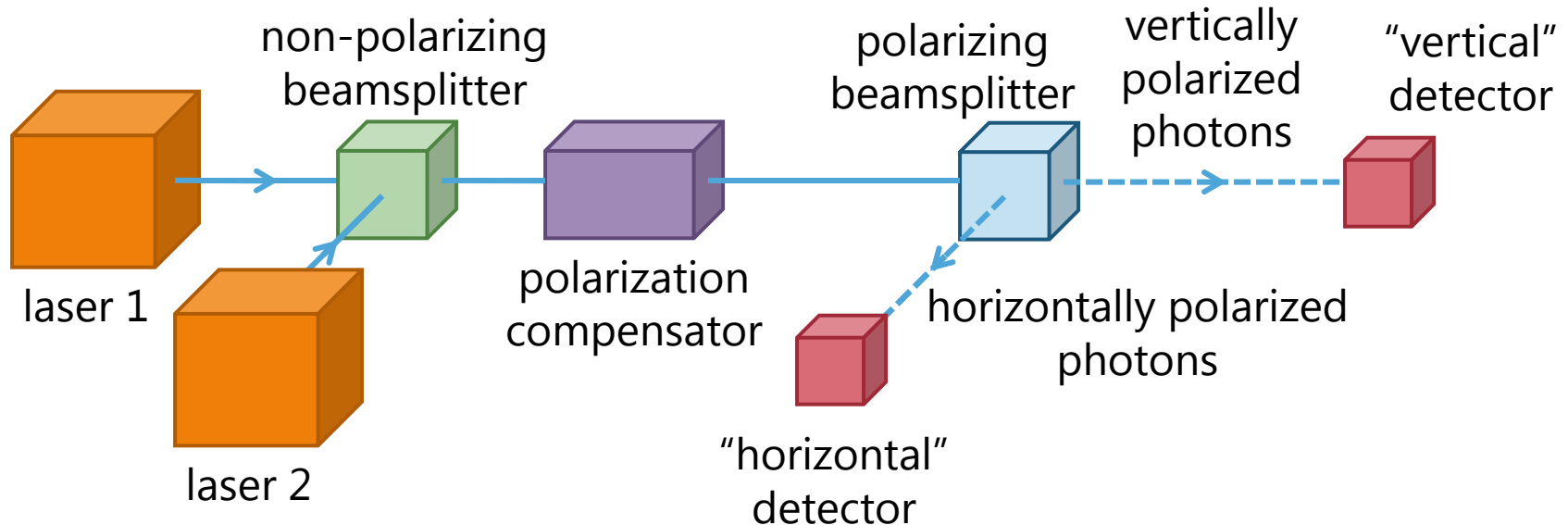
Presume laser 1 contributes a fraction  $P_1$  of the photons

and laser 2 contributes a fraction  $P_2$



# Mixed states

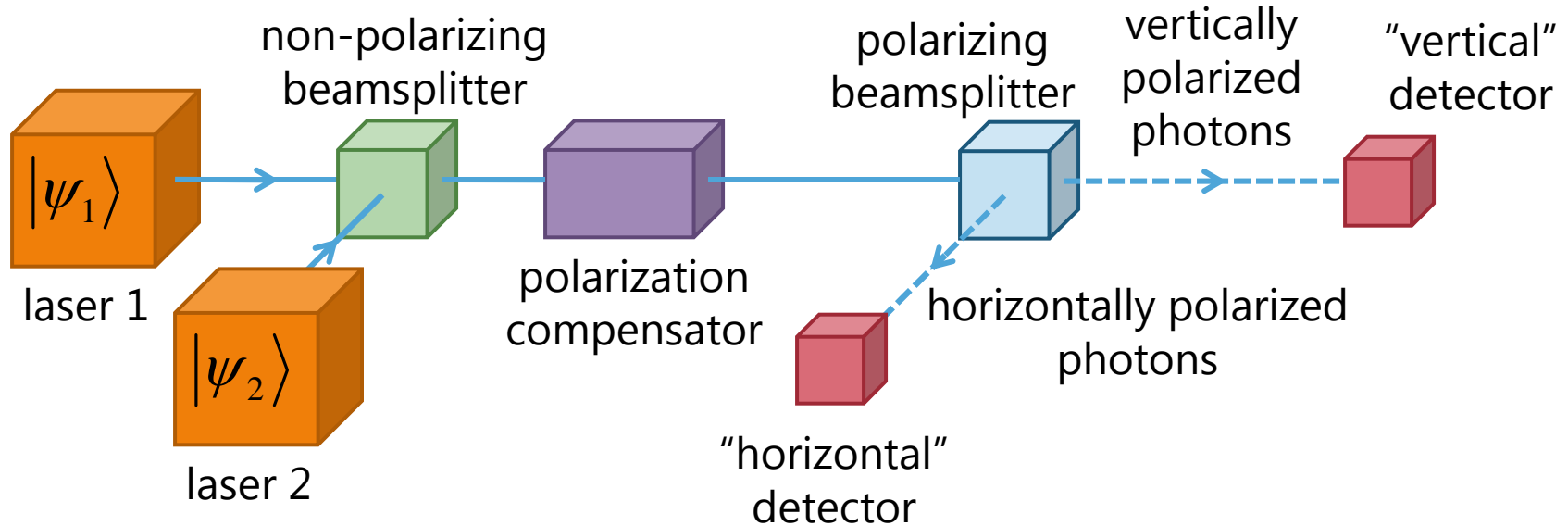
Then the probability a given photon is from laser 1 is  $P_1$   
and similarly there is probability  $P_2$  it is from laser 2



# Mixed states

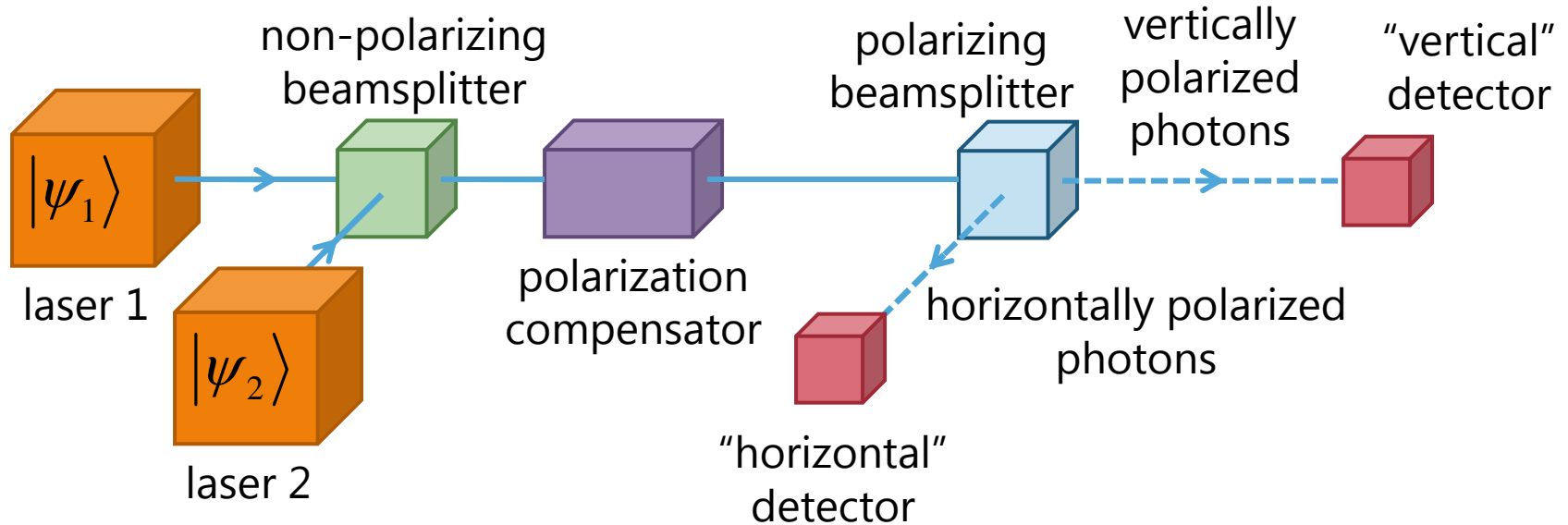
Presume also that these two lasers give uncorrelated photons  
of two possibly different polarization states

$|\psi_1\rangle$  and  $|\psi_2\rangle$  respectively



# Mixed states

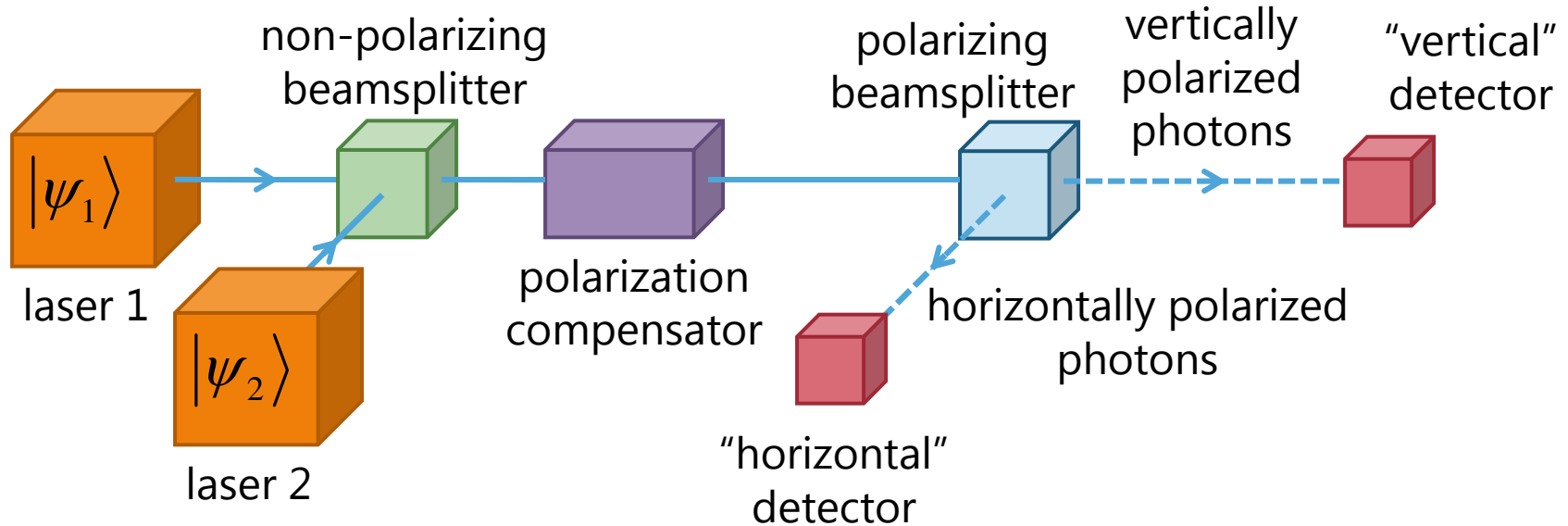
There is now no one setting of the compensator  
that in general will pass all the photons from both lasers  
to the vertical detector



# Mixed states

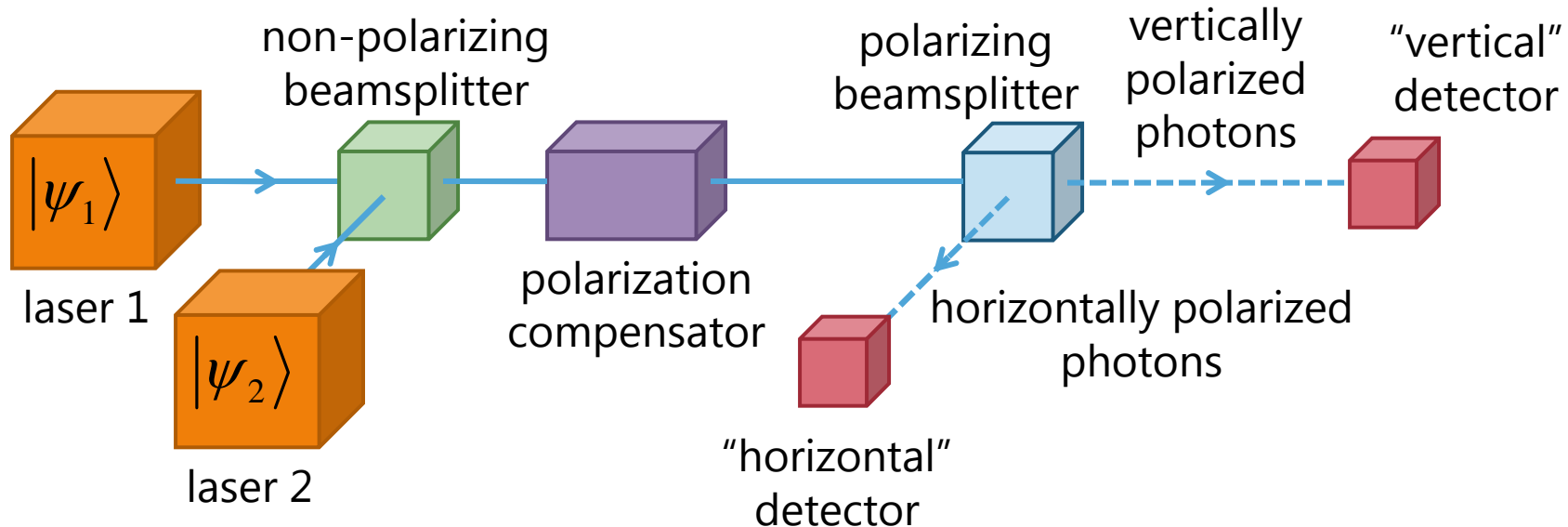
Hence, we cannot simply write this state

as some linear combination such as  $b_1|\psi_1\rangle + b_2|\psi_2\rangle$   
of the two different polarization states



# Mixed states

If we were able to do that, we could construct a  
polarizing filter  
to pass 100% of the photons

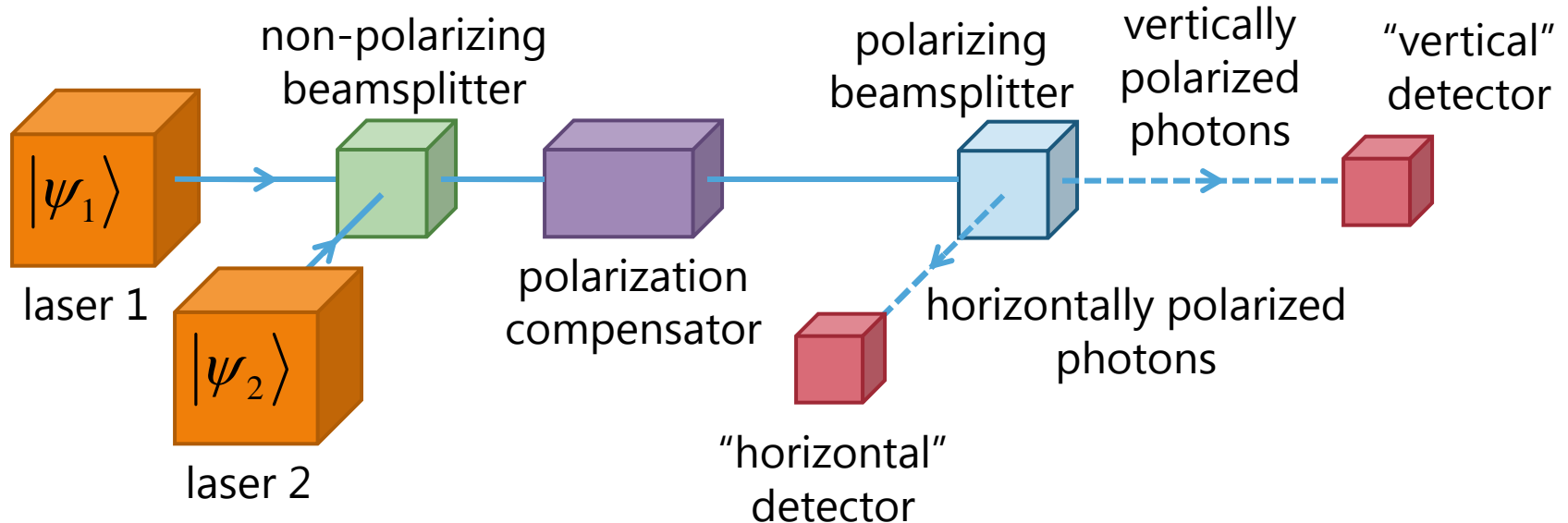


# Mixed states

So the state of these photons is described differently

as a "mixed state"

in contrast to a "pure state" like  $|\psi\rangle = a_H |H\rangle + a_V |V\rangle$



# Pure states for potential wells

Suppose, for some particle with mass

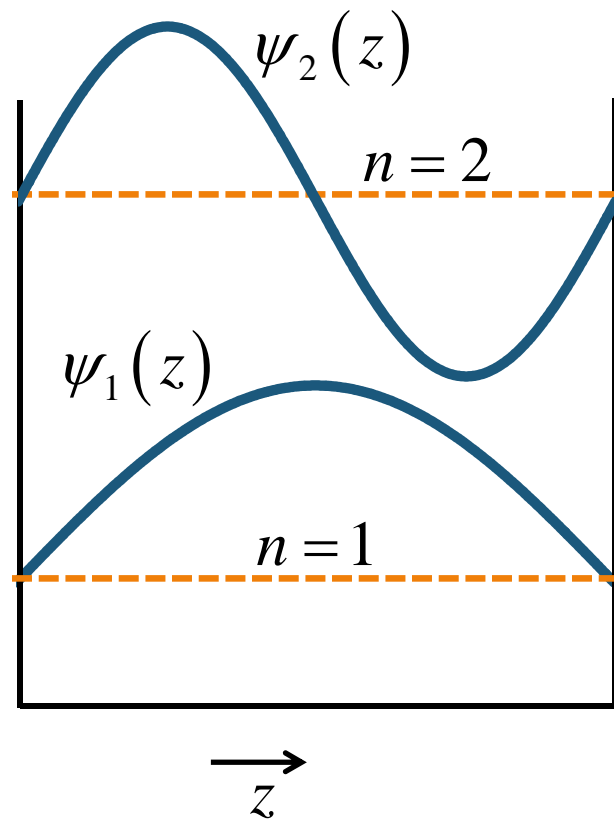
we have a potential well

such as the “infinite” one-dimensional potential well

We put it in a pure state

that is an equal linear superposition of the lowest two states of this well

$$|\psi\rangle = (1/\sqrt{2})(|\psi_1\rangle + |\psi_2\rangle)$$





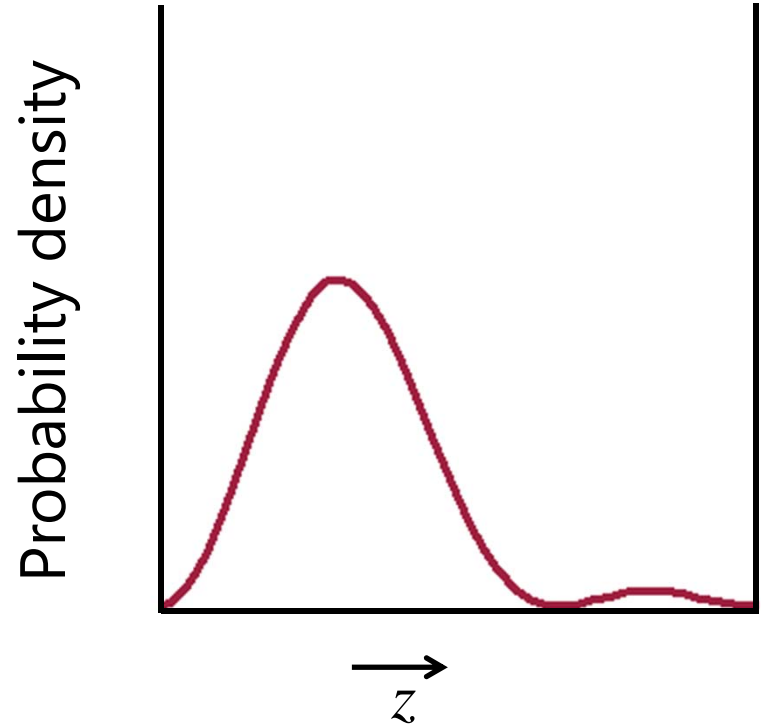
# Pure states for potential wells

In such a superposition

$$|\psi\rangle = \left(1/\sqrt{2}\right)(|\psi_1\rangle + |\psi_2\rangle)$$

the position of this particle  
will oscillate back and  
forwards

because of the different  
time-evolution factors  
for the two energy  
eigenstates



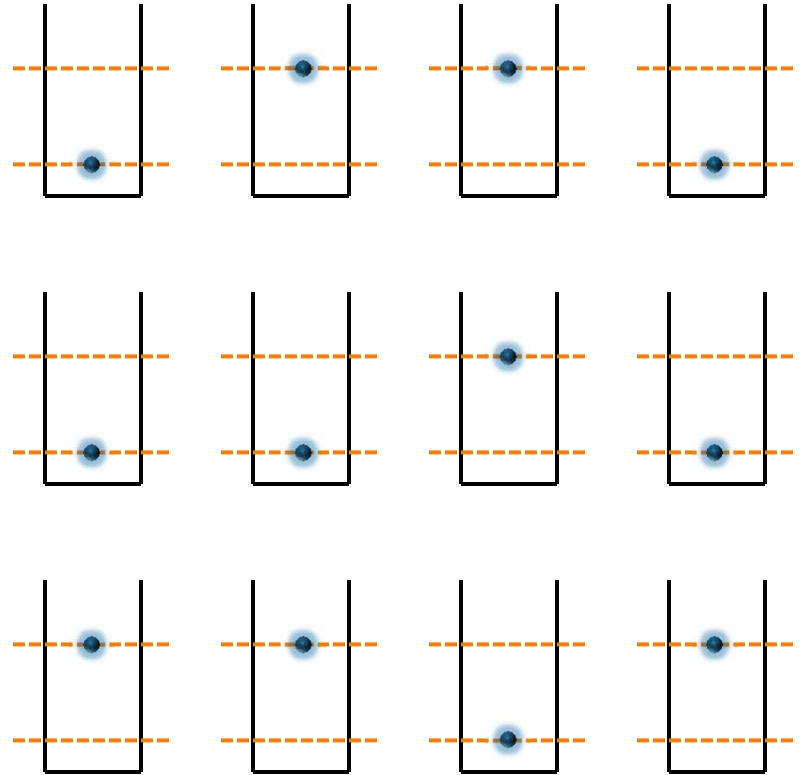
# Mixed states for potential wells

Suppose instead we take an ensemble of identical potential wells

and randomly prepare

half of them with the  
particle in the lowest state

and half of them with the  
particle in the second  
state

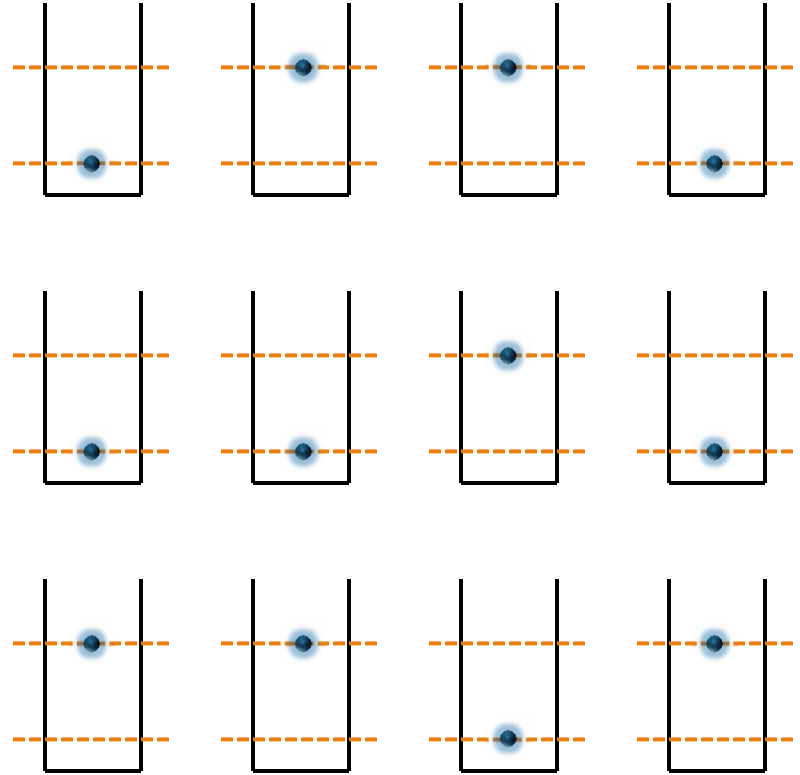


# Mixed states for potential wells

Statistically, since we do not know which wells are which  
at least before performing  
any measurements

each of these wells is in a  
mixed state

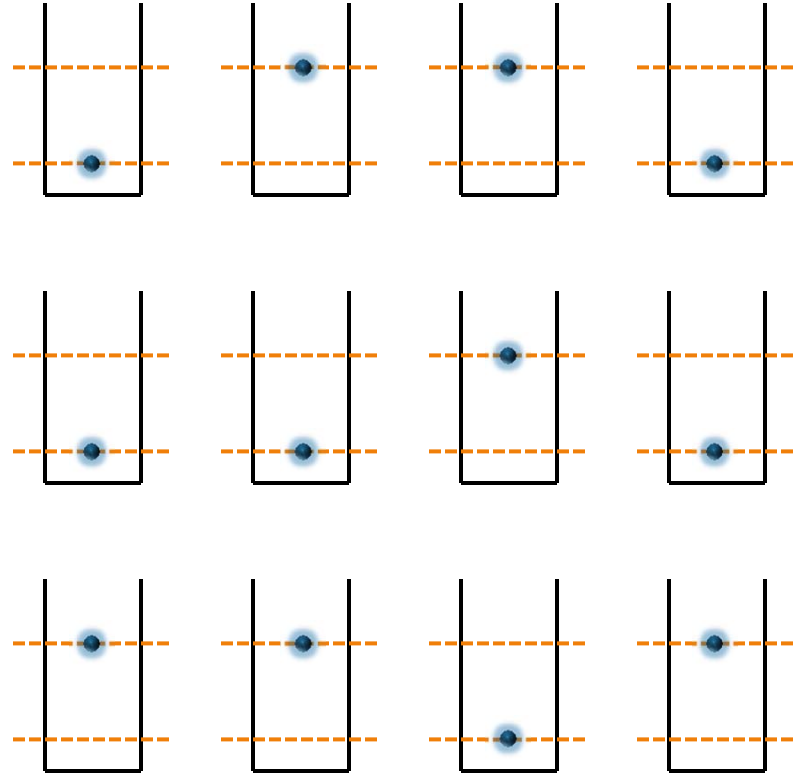
with 50% probability of  
being in either the first or  
second state



# Mixed states for potential wells

Now we evaluate the expectation value  $\langle z \rangle$  of the  $\hat{z}$  position operator for each potential well

In each well  $\langle z \rangle$  evaluates to the position of the center of the well since each of these wavefunctions is equally balanced about the center



# Mixed states for potential wells

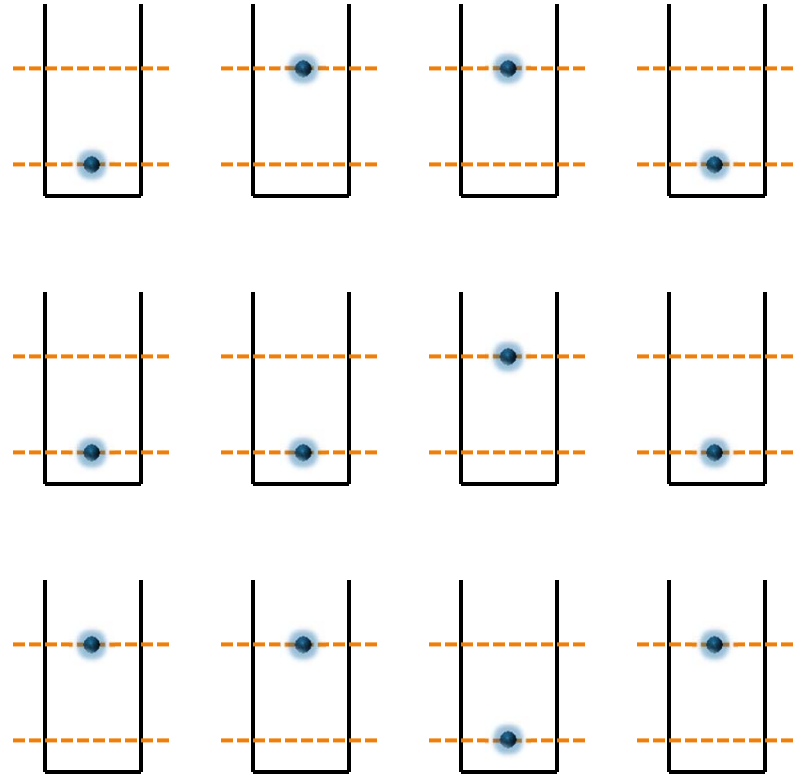
The “ensemble average”  $\overline{\langle z \rangle}$   
of expectation values from  
the different wells

is also zero

and there is no oscillation  
in time

Again it would not be correct  
simply to write the mixed  
state

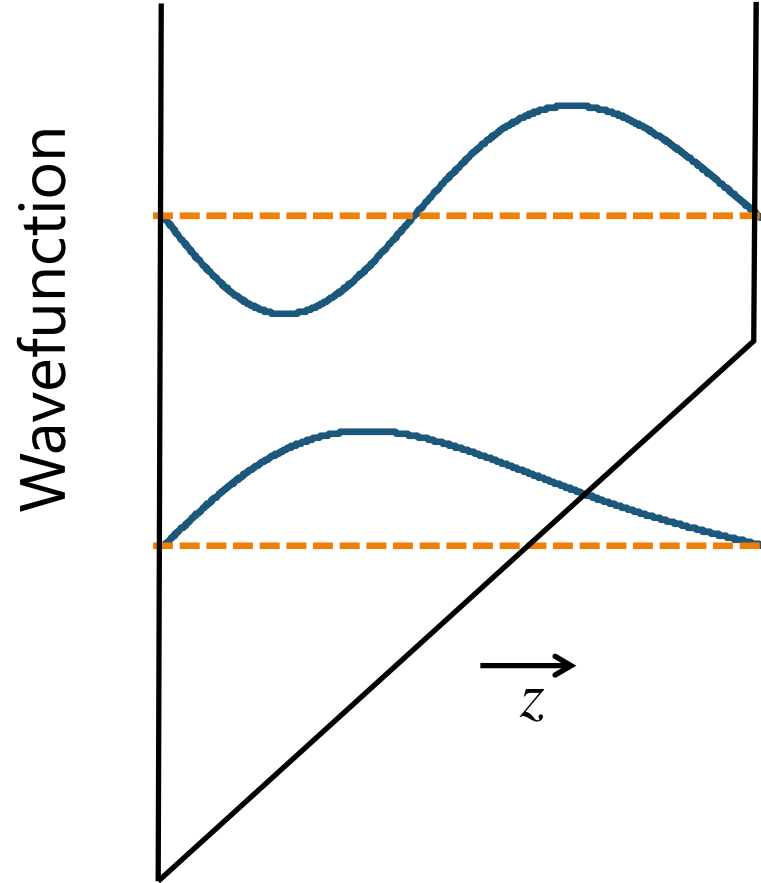
as a linear combination of the  
form  $b_1|\psi_1\rangle + b_2|\psi_2\rangle$



# Pure state in skewed wells

Suppose each well is skewed  
by applying electric field in the  
 $z$  direction  
for a particle like an electron  
in the well

Then  $\langle z \rangle$  is different for the first  
and second states of the well  
with  $\langle z \rangle = z_1$  for the first state  
and  $\langle z \rangle = z_2$  for the second state  
For the pure state, we still expect  
oscillation



# Mixed states for skewed wells

For a mixed state

with probabilities  $P_1$  and  $P_2$   
respectively that

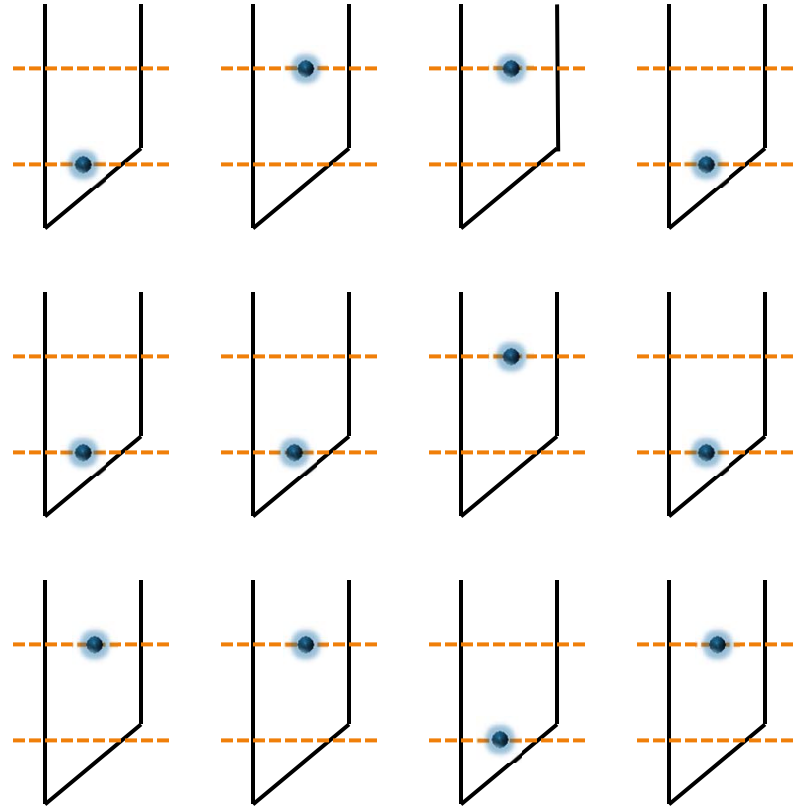
we had prepared a given well  
in the first or second state

we would still have no oscillation

The ensemble average value of  
the measured position

would now be

$$\overline{\langle z \rangle} = P_1 z_1 + P_2 z_2 \equiv \sum_{j=1}^2 P_j \langle \psi_j | \hat{z} | \psi_j \rangle$$



# Mixed state ensemble average expectation value

Generalizing from  $\overline{\langle z \rangle} = P_1 z_1 + P_2 z_2 \equiv \sum_{j=1}^2 P_j \langle \psi_j | \hat{z} | \psi_j \rangle$

we expect the ensemble average expectation value  
for some operator  $\hat{A}$  corresponding to an  
observable quantity

can be written  $\overline{\langle A \rangle} = \sum_j P_j \langle \psi_j | \hat{A} | \psi_j \rangle$

for some set of different quantum mechanical  
state preparations  $|\psi_j\rangle$

made with respective probabilities  $P_j$



# Mixed states

In considering mixed states

where we are saying that the quantum mechanical state could be any of a set of different possibilities  $|\psi_j\rangle$

with respective probabilities  $P_j$

the different  $|\psi_j\rangle$  need not be orthogonal

For example, we could be considering several different polarization states close to one another in angle

perhaps from some fluctuation in time in the precise output polarization of some laser

giving a mixed state of many different possible similar but not identical polarizations

# Density operator

However we are going to represent the mixed state

it must obviously contain the probabilities  $P_j$

and the pure states  $|\psi_j\rangle$

but it must not simply be a linear combination  
of the states

The structure we propose instead is the density operator

$$\rho = \sum_j P_j |\psi_j\rangle\langle\psi_j|$$

This is an operator because

it contains the outer products  $|\psi_j\rangle\langle\psi_j|$  of state vectors

# Density operator

In  $\rho = \sum_j P_j |\psi_j\rangle\langle\psi_j|$

we deliberately leave the “hat” off this operator  
to emphasize that its physical meaning and use  
are quite different from other operators we have  
considered

$\rho$  is not an operator representing some physical  
observable

Rather,  $\rho$  is representing the state  
in general, a mixed state  
of the system

# Density operator

If  $\rho$  is a useful way of representing the mixed state

it must allow us to calculate quantities like

the ensemble average measured value  $\overline{\langle A \rangle}$

for any physical observable with operator  $\hat{A}$

If we can evaluate  $\overline{\langle A \rangle}$  for such any physical observable

then  $\rho$  will be the most complete way we can have of describing this mixed quantum mechanical state

because it will tell us the value we will get of any measurable quantity

to within our underlying statistical uncertainties

# Density matrix and ensemble average values

To understand the properties of the density operator

we write it in terms of a complete orthonormal basis  $|\phi_m\rangle$

First we expand each of the pure states  $|\psi_j\rangle$  in this set

obtaining 
$$|\psi_j\rangle = \sum_u c_u^{(j)} |\phi_u\rangle$$

Then we use this expansion and its adjoint

in our definition  $\rho = \sum_j P_j |\psi_j\rangle \langle \psi_j|$  to obtain

$$\rho = \sum_j P_j \left( \sum_u c_u^{(j)} |\phi_u\rangle \right) \left( \sum_v (c_v^{(j)})^* \langle \phi_v| \right) = \sum_{u,v} \left( \sum_j P_j c_u^{(j)} (c_v^{(j)})^* \right) |\phi_u\rangle \langle \phi_v|$$

# Density matrix and ensemble average values

Written  $\rho = \sum_{u,v} \left( \sum_j P_j c_u^{(j)} \left( c_v^{(j)} \right)^* \right) |\phi_u\rangle \langle \phi_v| \equiv \sum_{u,v} \rho_{uv} |\phi_u\rangle \langle \phi_v|$

the matrix representation of  $\rho$  is now clear

We have for a matrix element in this basis

$$\rho_{uv} \equiv \langle \phi_u | \rho | \phi_v \rangle = \sum_j P_j c_u^{(j)} \left( c_v^{(j)} \right)^* \equiv \overline{c_u c_v^*}$$

Here we have also introduced and defined the idea of

the ensemble average of the coefficient product  $\overline{c_u c_v^*}$

We now usually talk of  $\rho$  as the density matrix

with matrix elements  $\rho_{uv}$

# Properties of the density matrix

We can deduce several properties from our definition of the density matrix

First, the density matrix is Hermitian

**Explicitly**  $\rho_{vu} \equiv \sum_j P_j c_v^{(j)} \left( c_u^{(j)} \right)^* = \left( \sum_j P_j c_u^{(j)} \left( c_v^{(j)} \right)^* \right)^* = \rho_{uv}^*$

Because the density matrix is Hermitian

so also is the density operator

since the density matrix is just a  
representation of the density operator

# Properties of the density matrix

Second, the diagonal elements  $\rho_{mm}$   
give us the probabilities of finding the system in a  
specific one of the states  $|\phi_m\rangle$

$c_m^{(j)} (c_m^{(j)})^* \equiv |c_m^{(j)}|^2$  is the probability for a pure state  $j$   
that we will find the system in state  $m$

Hence adding these up with probabilities  $P_j$   
gives the overall probability of finding the  
system in state  $m$  in the mixed state

(The off-diagonal elements are a measure of the  
"coherence" between different states and we will return  
to discuss this later)



# Properties of the density matrix

Third, the sum of the diagonal elements of the density matrix is unity

i.e., remembering that we can formally write the sum of the diagonal elements of some matrix or operator as the trace ( $Tr$ ) of the matrix or operator

$$Tr(\rho) = \sum_m \rho_{mm} = \sum_m \sum_j P_j |c_m^{(j)}|^2 = \sum_j P_j \sum_m |c_m^{(j)}|^2 = \sum_j P_j = 1$$

because the state  $|\psi_j\rangle$  is normalized (so  $\sum_m |c_m^{(j)}|^2 = 1$ )

and the sum of all the probabilities  $P_j$  of the various states  $|\psi_j\rangle$  in the mixed state must be 1

# Ensemble average value from the density matrix

Consider an operator  $\hat{A}$  for some physical observable  
and specifically consider the product  $\rho\hat{A}$

$$\rho\hat{A} = \sum_{u,v} \left( \sum_j P_j c_u^{(j)} \left( c_v^{(j)} \right)^* \right) |\phi_u\rangle \langle \phi_v| \hat{A}$$

We can therefore write some diagonal element of the resulting matrix as

$$\begin{aligned} \langle \phi_q | \rho\hat{A} | \phi_q \rangle &= \sum_{u,v} \left( \sum_j P_j c_u^{(j)} \left( c_v^{(j)} \right)^* \right) \langle \phi_q | \phi_u \rangle \langle \phi_v | \hat{A} | \phi_q \rangle \\ &= \sum_{u,v} \left( \sum_j P_j c_u^{(j)} \left( c_v^{(j)} \right)^* \right) \delta_{qu} \langle \phi_v | \hat{A} | \phi_q \rangle = \sum_v \sum_j P_j c_q^{(j)} \left( c_v^{(j)} \right)^* \langle \phi_v | \hat{A} | \phi_q \rangle \end{aligned}$$

# Ensemble average value from the density matrix

Then the sum of the all of these diagonal elements

$$\langle \phi_q | \rho \hat{A} | \phi_q \rangle = \sum_v \sum_j P_j c_q^{(j)} \left( c_v^{(j)} \right)^* \langle \phi_v | \hat{A} | \phi_q \rangle$$

is 
$$\sum_q \langle \phi_q | \rho \hat{A} | \phi_q \rangle = \sum_j P_j \left( \sum_v \left( c_v^{(j)} \right)^* \langle \phi_v | \right) \hat{A} \left( \sum_q c_q^{(j)} | \phi_q \rangle \right)$$
$$= \sum_j P_j \langle \psi_j | \hat{A} | \psi_j \rangle$$

Note this is the same as the ensemble average value  $\overline{\langle A \rangle}$   
of the expectation value of the operator  $\hat{A}$   
for this mixed state, as written before

# Ensemble average value from the density matrix

Hence we have a key result of density matrix theory

$$\overline{\langle A \rangle} = \text{Tr}(\rho \hat{A})$$

The density matrix can be used to deduce any measurable ensemble average property of a mixed state

Hence the density matrix gives a full description of a mixed state

Note that this result

is independent of the basis used to calculate the trace

The basis  $|\phi_m\rangle$  could be any set

that is complete for the problem of interest

# Ensemble average value from the density matrix

Note also that

if we have the system in a pure state  $|\psi\rangle$

in which case  $P = 1$  for that state

and is zero for any other pure state

then we recover the usual result for the expectation value

i.e., 
$$\text{Tr}(\rho \hat{A}) = \langle \psi | \hat{A} | \psi \rangle = \langle A \rangle$$

so the density matrix description gives the correct answers for pure or mixed states

# Time-evolution of the density matrix

We can directly calculate the time-evolution of the density matrix

We start with the Schrödinger equation for any particular one of the pure states in our mixed state

i.e.,  $\hat{H}|\psi_j\rangle = i\hbar \frac{\partial}{\partial t}|\psi_j\rangle$

and we substitute using  $|\psi_j\rangle = \sum_u c_u^{(j)}|\phi_u\rangle$

to obtain 
$$i\hbar \sum_n \frac{\partial c_n^{(j)}(t)}{\partial t} |\phi_n\rangle = \sum_n c_n^{(j)}(t) \hat{H} |\phi_n\rangle$$

Here all the time dependence of the state is in the  $c_n^{(j)}(t)$

# Time-evolution of the density matrix

Now operating from the left with  $\langle \phi_m |$

we have 
$$\langle \phi_m | i\hbar \sum_n \frac{\partial c_n^{(j)}(t)}{\partial t} | \phi_n \rangle = \langle \phi_m | \sum_n c_n^{(j)}(t) \hat{H} | \phi_n \rangle$$

i.e., 
$$i\hbar \frac{\partial c_m^{(j)}(t)}{\partial t} = \sum_n c_n^{(j)}(t) H_{mn}$$

where 
$$H_{mn} = \langle \phi_m | \hat{H} | \phi_n \rangle$$

is a matrix element of the Hamiltonian

# Time-evolution of the density matrix

We can take the complex conjugate of both sides of

$$i\hbar \frac{\partial c_m^{(j)}(t)}{\partial t} = \sum_n c_n^{(j)}(t) H_{mn}$$

Noting that  $\hat{H}$  is Hermitian, i.e.,  $H_{mn}^* = H_{nm}$  we have

$$-i\hbar \frac{\partial \left( c_m^{(j)}(t) \right)^*}{\partial t} = \sum_n \left( c_n^{(j)}(t) \right)^* H_{nm}$$

or trivially changing indices

$$-i\hbar \frac{\partial \left( c_n^{(j)}(t) \right)^*}{\partial t} = \sum_s \left( c_s^{(j)}(t) \right)^* H_{sn}$$



# Time-evolution of the density matrix

But from our previous result for

the elements of the density matrix  $\rho_{uv} = \sum_j P_j c_u^{(j)} \left( c_v^{(j)} \right)^*$

we can take the time derivative to obtain

$$\frac{\partial \rho_{mn}}{\partial t} = \sum_j P_j \left( c_m^{(j)} \frac{\partial \left( c_n^{(j)} \right)^*}{\partial t} + \left( c_n^{(j)} \right)^* \frac{\partial c_m^{(j)}}{\partial t} \right)$$

Now we can substitute using our previous results

$$i\hbar \frac{\partial c_m^{(j)}(t)}{\partial t} = \sum_q c_q^{(j)}(t) H_{mq} \quad -i\hbar \frac{\partial \left( c_n^{(j)}(t) \right)^*}{\partial t} = \sum_s \left( c_s^{(j)}(t) \right)^* H_{sn}$$

(We changed the summation index to  $q$  in the first result)

# Time-evolution of the density matrix

Hence  $\frac{\partial \rho_{mn}}{\partial t} = \sum_j P_j \left( c_m^{(j)} \frac{\partial (c_n^{(j)})^*}{\partial t} + (c_n^{(j)})^* \frac{\partial c_m^{(j)}}{\partial t} \right)$  becomes

$$\begin{aligned} \frac{\partial \rho_{mn}}{\partial t} &= \sum_j P_j \left( \frac{i}{\hbar} c_m^{(j)} \sum_q (c_q^{(j)})^* H_{qn} - \frac{i}{\hbar} (c_n^{(j)})^* \sum_s c_s^{(j)} H_{ms} \right) \\ &= \frac{i}{\hbar} \left\{ \sum_q \left[ \sum_j P_j c_m^{(j)} (c_q^{(j)})^* \right] H_{qn} - \sum_s H_{ms} \left[ \sum_j P_j c_s^{(j)} (c_n^{(j)})^* \right] \right\} \end{aligned}$$

Note, though, that by definition  $\rho_{uv} \equiv \sum_j P_j c_u^{(j)} (c_v^{(j)})^*$

so we can substitute for the terms in [ ... ]

# Time-evolution of the density matrix

Hence we have

$$\frac{\partial \rho_{mn}}{\partial t} = \frac{i}{\hbar} \left( \sum_q \rho_{mq} H_{qn} - \sum_s H_{ms} \rho_{sn} \right) = \frac{i}{\hbar} \left( (\rho \hat{H})_{mn} - (\hat{H} \rho)_{mn} \right) = \frac{i}{\hbar} [\rho, \hat{H}]_{mn}$$

Since this is true for every matrix element  $mn$

we have

$$\frac{\partial \rho}{\partial t} = \frac{i}{\hbar} [\rho, \hat{H}]$$

which tells us how the mixed state evolves in time  
and is a key result for the density matrix