For this formula, one finds that if $ka < 1$ there is very little angular dependence; plots for $ka > 1$ are in Branden. This concludes our discussion of scattering.

THE DENSITY MATRIX: QUANTUM STATISTICS

The last major topic of this course will be finding a way to represent two kinds of uncertainty:

1. In quantum mechanics, even if we know a wave function $\Psi(t)$ perfectly, the results of measurement will be unpredictable if $\Psi$ is not an eigenstate of the measured operator.

2. In classical "statistical physics," we often have to use probability to reflect our ignorance about the actual microscopic state. For example, in a system at nonzero temperature $T$, the probability of the system being in microstate $j$ with energy $E_j$ is proportional to $e^{-E_j/k_B T}$. 
Previously in QM a state has been represented as a vector in a "complex linear vector space" (Hilbert space). We can specify a state by giving its coefficients over any basis. For an orthonormal basis like we normally use, this representation might look like

\[ |\Psi\rangle = \sum_{i} c_i |\Psi_i\rangle + c_2 |\Psi_2\rangle + \ldots \]

where \( |\Psi_i\rangle \) are the basis states, \( i = 0, 1, \ldots, N \) and

\[
\sum_{i=0}^{N} |c_i|^2 = 1.
\]

We refer to such a state \( |\Psi\rangle \) as a **pure state**: we know the exact QM state of the system, although some measurements may involve probability if the state \( |\Psi\rangle \) is not an eigenstate (of the measured operator).

In the following we will instead describe states by a **density matrix** (which takes on especially simple form for a pure state). This will enable us to understand states that are not pure states.
An example of a mixed state is the following (see below) consider a single spin $-\frac{1}{2}$ degree of freedom.

Our basis should have two orthonormal states, which we take to be $|\uparrow\rangle$ and $|\downarrow\rangle$.

Example of pure states:

$|\uparrow\rangle$ spin is polarized along $\hat{z}$

$|\downarrow\rangle$ spin points along $-\hat{z}$

$\phi_x = \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}$ spin state points along $\hat{x}$

(this is an eigenstate of $S_x$, but not of $S_z$).

A mixed state might be

"$|\uparrow\rangle$ with probability $\frac{1}{2}$, and $|\downarrow\rangle$ with probability $\frac{1}{2}$".

The meaning of probability here is as if I had flipped a coin but not yet looked to see whether it came up heads or tails: in a mixed state one doesn't know the microscopic QM state. We can figure out the results of experiment on this mixed state:
if the mixed state is

\[ |\uparrow\rangle \text{ with prob. } \frac{1}{2} \text{ and } |\downarrow\rangle \text{ with prob. } \frac{1}{2}, \]

measuring \( S_z \) gives:

\[ + \frac{1}{2} \text{ with prob. } \frac{1}{2}, \quad - \frac{1}{2} \text{ with prob. } \frac{1}{2} \]

measuring \( S_x \) gives:

\[ (+ \frac{1}{2}, - \frac{1}{2}) \text{ with prob. } \frac{1}{4}, \quad (+ \frac{1}{2}, - \frac{1}{2}) \text{ with prob. } \frac{1}{4} \]

or overall \( S_x \) gives

\[ \frac{1}{2} \text{ with prob. } \frac{1}{2}, \quad - \frac{1}{2} \text{ with prob. } \frac{1}{2}. \]

Note that this mixed state gives the same \( S_z \) result as \( \frac{1}{\sqrt{2}} |\uparrow\rangle + \frac{1}{\sqrt{2}} |\downarrow\rangle \), but a different result for \( S_x \) than \( \frac{1}{\sqrt{2}} |\uparrow\rangle + \frac{1}{\sqrt{2}} |\downarrow\rangle \) gave.

Can we formalize the difference between mixed states and pure states, and find an example for writing both? Let's start with pure state \( |\uparrow\rangle \).

Suppose we start with that \( |\uparrow\rangle \) is one of my basis states: then I define the density matrix \( \rho \) to be the matrix with \( 1 \) at element \( ij \), and 0 elsewhere:

\[
\rho = \begin{pmatrix}
0 & 0 \\
0 & 1
\end{pmatrix}
\]
Now suppose that I have an operator $\hat{\sigma}$. This operator is represented in the fixed basis by a matrix: the elements of this matrix $M$ are

$$
M_{ij} = \langle \psi_i | \hat{\sigma} | \psi_j \rangle, \quad i, j = 1, \ldots, N.
$$

In particular, the expectation value of $\hat{\sigma}$ in state $| \psi_j \rangle$ is $M_{jj}$. We can write $\hat{\sigma}$ abstractly as

$$
\hat{\sigma} = \left( \sum_i | \psi_i \rangle \langle \psi_i | \right) \delta^{ij} \left( \sum_j | \psi_j \rangle \langle \psi_j | \right)
$$

= identity operator
by completeness of basis

$$
= \sum_{i,j} | \psi_i \rangle \langle \psi_i | M_{ij} | \psi_j \rangle \langle \psi_j |.
$$

Using this idea for the density matrix we just wrote down for the pure state $| \psi_j \rangle$, we see that it corresponds to an operator

$$
\hat{\sigma} = | \psi_j \rangle \langle \psi_j | \quad \text{(density operator for state } | \psi_j \rangle \text{)}.
$$
The density operator for a pure state can be used to get results of experiments:

\[ \hat{\rho} = \sum_j \vert \psi_j \rangle \langle \psi_j \vert \]

Now \[ \langle \psi_j \vert \psi_i \rangle = \delta_{ij} \] by orthonormality of the basis, so

\[ \hat{\rho} = \sum_j \vert \psi_j \rangle \langle \psi_j \vert \]

\[ \hat{\rho} = 1_{\mathcal{H}} \]

We define the trace of an operator \( \hat{O} \) as

\[ \text{Tr} \hat{O} = \sum_i \langle \psi_i \vert \hat{O} \vert \psi_i \rangle \]

where \( \psi_i \) form an orthonormal basis; note that \( \text{Tr} \hat{O} = \) matrix trace (sum of diagonal elements) of the matrix that represents \( \hat{O} \) in this basis. It is an important fact of linear algebra that the trace is basis-independent.

Finally,

\[ \text{Tr} (\hat{\rho} \hat{\sigma}) = \sum_i \langle \psi_i \vert \hat{\rho} \hat{\sigma} \vert \psi_i \rangle = \sum_i \delta_{ij} \langle \psi_i \vert \hat{\sigma} \vert \psi_j \rangle = \langle \psi_j \vert \hat{\tau} \vert \psi_j \rangle \]
We have shown in one basis that $\text{Tr}(\rho \delta) =$
the expectation value of $\delta$ in the pure state defined by $\delta$,
but since trace is basis-independent, this works
in any basis.

In general, the matrix representation of $\rho$ for a pure
state $|\psi_j\rangle$ will be more complicated (and not diagonal) in
a basis where $|\psi_j\rangle$ is not an eigenstate,
but soon we will see that it is possible to
make a basis-independent test for pure states.

What about mixed states? Since

$$\rho = \sum_a |\psi_a\rangle \langle \psi_a|$$

we define $\rho = \sum_a |\psi_a\rangle \langle \psi_a| W_a < \psi_a |$ for a
mixed state, where $W_a$ are probabilities for
different pure state $|\psi_a\rangle$ (not necessarily
orthogonal). A pure state density matrix
contains one state $\psi$ with $W_\psi = 1$, while
a mixed state density matrix has multiple states.
Suppose we use our previous formula for $<\hat{O}>$:

\[
<\hat{O}> = \text{Tr} (\hat{\rho} \hat{O})
\]

\[
= \text{Tr} \left( \sum_{\alpha} |\alpha> <\alpha| \hat{O} \right)
\]

\[
= \sum_{i,\alpha} |\psi_{i} \chi_{\alpha}> <\alpha | \hat{O} | \psi_{i} \chi_{\alpha}>
\]

\[
= \sum_{\alpha} \chi_{\alpha} \left( \sum_{i} |\psi_{i} \chi_{\alpha}> <\alpha | \hat{O} | \psi_{i} \chi_{\alpha}>ight)
\]

\[
= \sum_{\alpha} \chi_{\alpha} \left( \text{Tr} (\hat{\rho}_{\alpha} \hat{O}) \right)
\]

where $\hat{\rho}_{\alpha}$ is the density matrix for pure state $\alpha$. As an example of the matrix rep. for a mixed state, consider the "half up and half down" state of a spin-1/2:

\[
\hat{\rho} = \frac{1}{2} \left( \begin{array}{cc} 1 & \downarrow \uparrow <\uparrow |\downarrow > <\downarrow |\uparrow > \\ \downarrow <\uparrow |\downarrow > <\downarrow |\uparrow > & \frac{1}{2} \end{array} \right)
\]

in the $S_{2}$ basis.

Now we can see that this density matrix is not that of any pure state since $\hat{\rho}^{2} = \frac{\hat{\rho}}{2} \neq \hat{\rho}$.

Also, since $\hat{\rho} = \frac{1}{2} \mathbb{I}$, under a unitary transformation

\[
\hat{\rho} \rightarrow U \hat{\rho} U^{-1} = \frac{1}{2} U \mathbb{I} U^{-1} = \frac{1}{2} \mathbb{I} = \hat{\rho}
\]

so this particular $\hat{\rho}$ is basis-independent.
So for pure states we have $\hat{\rho} = |\gamma\rangle\langle\gamma|$ and get expectation values of observables $\hat{O}$ via 
$\langle \hat{O} \rangle = \langle \gamma \left| \hat{O} \right| \gamma \rangle = Tr(\hat{\rho} \hat{O})$.

The trace is basis-independent. To get a simple matrix rep. for $\hat{\rho}$, note that in an orthonormal basis with $|\gamma\rangle = |\gamma\rangle$, $\hat{\rho}$ is the matrix 
\[
\begin{pmatrix}
1 & 0 \\
0 & 0 \\
\end{pmatrix}
\]
We see in this basis that $Tr \hat{\rho} = 1$ and that $\hat{\rho}^2 = \hat{\rho}$. (The second statement is basis-independent since under a unitary transformation $\gamma \rightarrow U\gamma$, $\hat{\rho} \rightarrow U \hat{\rho} U^{-1}$ and $\hat{\rho}^2 \rightarrow (U \hat{\rho} U^{-1})(U \hat{\rho} U^{-1}) = U \hat{\rho}^2 U^{-1}$.)

A mixed state is made up of multiple pure states $|\alpha\rangle$ with probabilities $W_\alpha$, $\alpha = 1, \ldots, M$. $\sum_\alpha W_\alpha = 1$.

We define the density operator to be 
\[
\hat{\rho} = \sum_\alpha |\alpha\rangle W_\alpha \langle \alpha|
\]
Note that the states need not be orthogonal.
Suppose we use our previous formula for $\langle \hat{\varphi} \rangle$:

\[
\langle \hat{\varphi} \rangle = \text{Tr} (\hat{\varphi} \hat{\varphi}) = \text{Tr} \left( \sum_{\alpha} \langle \alpha | W_\alpha \langle \alpha | \hat{\varphi} \rangle \right) = \sum_{\alpha} \langle \alpha | W_\alpha \left( \sum_i \langle \psi_i | \alpha \rangle \langle \alpha | \psi_i \rangle \right) \langle \psi_i | \alpha \rangle \langle \alpha | \hat{\varphi} \rangle \rangle \rangle = \sum_{\alpha} W_\alpha \left( \text{Tr} (\hat{\varphi} \hat{\varphi}) \right)
\]

where $\hat{\varphi}_\alpha$ is the density matrix for pure state $\alpha$. As an example of the matrix rep. for a mixed state, consider the "half up and half down" state of a spin-$\frac{1}{2}$.

\[
\hat{\varphi} = \frac{1}{2} \left( \begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right) = \left( \begin{array}{cc} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{array} \right)
\]

in the $S_2$ basis.

Now we can see that this density matrix is not that of any pure state since $\hat{\varphi}^2 = \frac{\hat{\varphi}}{2} \neq \hat{\varphi}$.

Also, since $\hat{\varphi} = \frac{1}{2} I$, under a unitary transformation

\[
\hat{\varphi} \rightarrow U \hat{\varphi} U^{-1} = \frac{1}{2} U I U^{-1} = \frac{1}{2} I = \hat{\varphi}
\]

so this particular $\hat{\varphi}$ is basis-independent.
So for pure state we have \( \hat{\rho} = |\psi\rangle \langle \psi| \)
and get expectation values of observables \( \hat{O} \) via
\[
\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle = \text{Tr}(\hat{O} \hat{\rho}).
\]
The trace is basis-independent. To get a simple matrix rep. for \( \hat{\rho} \), note that in an orthonormal basis with \( |\psi_i\rangle = |\psi\rangle \) \( \hat{\rho} \) is the matrix
\[
\begin{pmatrix}
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
\]
We see in this basis that \( \text{Tr} \hat{\rho} = 1 \)
and that \( \hat{\rho}^2 = \hat{\rho} \).
(The second statement is basis-independent since under a unitary transformation \( U \), \( \hat{\rho} \rightarrow U \hat{\rho} U^{-1} \)
and \( \hat{\rho}^2 \rightarrow (U \hat{\rho} U^{-1})(U \hat{\rho} U^{-1}) = U \hat{\rho}^2 U^{-1} \).

A mixed state is made up of multiple pure states \( |\alpha\rangle \) with probabilities \( W_\alpha \), \( \alpha = 1, \ldots, M \).
\[
\sum_\alpha W_\alpha = 1.
\]
We define the density operator to be
\[
\hat{\rho} = \sum_\alpha |\alpha\rangle \langle \alpha| W_\alpha \rho_{\alpha}.K_{\alpha}|.\]
Note that the states need not be orthogonal.