The Density Matrix

Recall the two results of the assignment on “Matrix Calisthenics”:

\[
tr\{\hat{A}\hat{B}\} = tr\{\hat{B}\hat{A}\} \\
tr\{|\phi\rangle\langle\psi|\} = \langle\psi|\phi\rangle
\]

Definition

\[
tr\{\hat{\rho}\hat{A}\} = tr\{\hat{A}\hat{\rho}\} = tr\{\hat{A}|\psi\rangle\langle\psi|\} = \langle\psi|\hat{A}|\psi\rangle = \langle\hat{A}\rangle.
\]

Statistical mechanics

Define \( \hat{\rho}_i = |i\rangle\langle i| \). Clearly, the expectation value of \( \hat{A} \) in our so-called “mixed state” is

\[
\sum_i p_i \langle i|\hat{A}|i\rangle = \sum_i p_i tr\{\hat{\rho}_i\hat{A}\}
\]

but

\[
tr\{\hat{\rho}\hat{A}\} = tr\left\{\sum_i p_i \hat{\rho}_i\hat{A}\right\} = \sum_i p_i tr\{\hat{\rho}_i\hat{A}\}.
\]

The trace of the density matrix

\[
tr\{\hat{\rho}\} = tr\{\hat{\rho}\hat{1}\} = \langle\hat{1}\rangle = 1.
\]