Today Quantum Statistical Mechanics

and a comparison to classical probability theory

<table>
<thead>
<tr>
<th>Classical</th>
<th>Quantum statistical</th>
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<tbody>
<tr>
<td>prob. mass function $p_m$</td>
<td>Hilbert space $\mathcal{H}$, $N$-dim</td>
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<tr>
<td>$m = 1, 2, \ldots$</td>
<td>density operator $\rho : \mathcal{H} \to \mathcal{H}$</td>
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<tr>
<td>$\rho &gt; 0$ $\text{tr} \rho = 1$</td>
<td>$\rho &gt; 0$ for $\rho$ must be self-adjoint</td>
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</table>

Def the $\rho > 0$ means $\langle \psi | \rho | \psi \rangle > 0 \forall \psi \in \mathcal{H}$

But if $\rho > 0$ then $\rho$ must be self-adjoint — since always gives real inner products, real eigenvalues, is diagonalizable with ON eigenvectors

It follows from this that if $\rho$ is a density operator, then $\lambda_i > 0$ and $\sum \lambda_i = 1$

observable $f : \{1, \ldots, N\} \to \mathbb{R}$

$\mathbb{E}_\rho(f) = \sum_i f(i) p_i$

expected value of $f$

$\int f \rho = \cdots$ (Equation)

an observable is a self-adjoint operator $A : \mathcal{H} \to \mathcal{H}$

the expected value of $A$ wrt $\rho$ is $\mathbb{E}_\rho(A) = \text{tr}(A \rho)$

E.g. $A_\rho = \rho A$ can be diagonalized using $\text{tr}(A \rho) = \text{tr}(\rho A)$ the same basis

$A = \begin{pmatrix} \alpha_1 & \cdots & \alpha_n \end{pmatrix}$ $\rho = \begin{pmatrix} \lambda_1 & \cdots & \lambda_n \end{pmatrix}$

and then $\text{tr}(A \rho) = \text{tr}(\rho A) = \sum_i \alpha_i \lambda_i$ which is like the probability expected value in classical probability theory.

This is sort of a non-commutative probability theory.
Quantum mechanics

\[ \phi \]

\( \phi \) unit vector is called a state.

A density operator is called a state.

In general, \( \rho = (\lambda_1, \ldots, \lambda_n) \).

Eigenvalues \( \lambda_1, \ldots, \lambda_n \).

\[ \rho \rightarrow \Pi \rho \] is a density operator.

"a pure state"

\[ E_\phi(A) := \langle \phi | A | \rho \rangle \]

\[ \text{tr} (A \Pi \rho) = \langle \phi | A | \rho \rangle \]

\[ \# \text{tr}(A | \rho \rangle \langle \rho |) = \text{tr}(\langle \phi | A | \phi \rangle) \]

= \langle \phi | A | \phi \rangle

Formulas for Traces

\[ \text{Def} \quad \text{tr} (A) = \sum_{i=1}^{N} \alpha_{ii} = \sum_{i=1}^{N} \langle \psi_i | A | \psi_i \rangle \]

1. \( \text{tr} (AB) = \text{tr} (BA) \neq \text{tr} A \times \text{tr} B \)

2. \( \text{tr} (A + B) = \text{tr} A + \text{tr} B \)

3. \( \text{tr} (A \otimes B) = \text{tr} A \times \text{tr} B \)

4. \( \text{tr} (A) \) invariant under orthonormal basis change

\[ \begin{align*}
\text{Eq. 1.} \quad \text{tr} (AB) & = \sum_{i=1}^{N} \langle \psi_i | AB | \psi_i \rangle \\
& = \sum_{i=1}^{N} \langle \psi_i | A | \psi_j \rangle \langle \psi_j | B | \psi_i \rangle \\
& = \sum_{i=1}^{N} \sum_{j=1}^{N} \langle \psi_i | A | \psi_j \rangle \langle \psi_j | B | \psi_i \rangle \\
& = \sum_{j=1}^{N} \sum_{i=1}^{N} \langle \psi_j | B | \psi_i \rangle \langle \psi_i | A | \psi_j \rangle = \text{tr} (BA)
\end{align*} \]
4. \( tr(U^*AU) = tr(UU^*A) = tr(A) \)

Eqn: \( tr(1\psi\psi^\dagger) = tr(\Phi(\Phi^\dagger)) \)

\( = tr(\langle\psi|\psi\rangle) = 1 \)

so trace of a pure state is 1

A density operator \( \rho \) is a pure state iff \( \rho^2 = \rho \)

\( \rho = |\psi\rangle\langle\psi| \) where \( \rho\phi = \phi \)

5. In general, any state is a convex combination of pure states.

\( \rho = (\lambda_1, \ldots, \lambda_n) \) with eigenstates \( \psi_1, \ldots, \psi_n \)

\[ \rho = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i| \]

// spectral theorem

\( \sum \lambda_i = 1 \), \( \lambda_i \geq 0 \) i.e. a convex combination

\[ E_\rho(A) = tr(\rho A) = \sum_i \lambda_i tr(A|\psi_i\rangle\langle\psi_i|) = \sum_i \langle\psi_i|A|\psi_i\rangle \lambda_i \]

In quantum mechanics, we only have \( \langle \psi | A | \psi \rangle \), but here we have many pure states.

Markov chain \( (X_n)_{n=0}^{\infty} \), \( \mu_0 \) initial distribution.

\[ \mu_t = E_{\mu_0}(X_t) = \sum_i \mu_0(i) P(i,j) \]

\[ \mu_0 \]

\[ \mu_t \]

\[ \mu_0 \]

\[ \mu_0 \]

\[ \mu_t \]

Quantum Statistical Dynamics \( \rho_0 \rightarrow \rho_t \)
Two kinds of dynamics — coherent and decoherent

Decoherent first

Let \( \mathcal{M}_n \) be a measurement, i.e., \( \sum\limits_{n=1}^{N} M_n^* M_n = I \)

\( M_n^* M_n \) is self-adjoint and hermitian observable

\( (AB)^* = B^* A^* \)

\( M_n^* M_n \) is called the event that \( n \) occurs

\( \rho \) is a density operator

\[ E_n (M_n^* M_n) = \text{tr} (M_n^* M_n \rho) = \text{probability that } n \text{ occurs} \]

\( \text{tr} (M_n^* \rho M_n) \)

If \( n \) occurs, then after the measurement, \( \rho \) becomes \( \rho' \)

\[ \rho' = \frac{M_n^* \rho M_n}{\text{tr} (M_n^* \rho M_n)} \]

after the measurement, if we forget the outcome, then

\[ \rho' = \sum_{n=1}^{N} M_n^* \rho M_n \]

Natural Dynamics

\( U(t) : \mathcal{H} \to \mathcal{H} \) unitary

\[ \psi_t = U(t) \psi_0 \]

\( A \) observable

\[ E_{\psi_0} (A) \equiv E_{\psi_0} (A_t) \] for \( A_t \)

\[ \langle \psi_t | A | \psi_t \rangle = \langle U(t) \psi_0 | A | U(t) \psi_0 \rangle = \langle \psi_0 | U^* (t) A U(t) | \psi_0 \rangle = \langle \psi_0 | A(t) | \psi_0 \rangle \Rightarrow A(t) = U^* (t) A(0) U(t) \]
Next \[ E_{\rho_0}(A_0) = E_{\rho}(A_0) \]
\[
= \text{tr}(A_0 \rho_0) = \text{tr}(A_0 \rho) \]
\[
= \text{tr}(U(t)^* A_0 U(t) \rho_0) = \text{tr}(U(t)^* A_0 U(t) \rho) \]
\[
\implies \rho = U(t)^* \rho_0 U(t) \]

for natural dynamics.

For real applications get both decoherence & natural dynamics

\[
\rho = \sum_{m=1}^{N} U M_m \rho M_m^* U^* \]

\[ \rho \in L(H) \rightarrow \rho \] operator

Define \[ L \rho = \sum_{m=2}^{N} U M_m \rho M_m^* U^* \]

\[ L : L(H) \rightarrow L(H) \text{ or } L \in L(L(H)) \]