Density Matrices

A Max Franklin Production

Defining a Density Matrix

If we consider an observable A in the state $|\psi\rangle$...

- The density matrix is the sum over all of the "pure states"
- This is mathematically defined as $\rho = \sum p_j |\psi_j\rangle\langle\psi_j|$
- In this format, the coefficients p_j are non negative and sum to one

For any pure state, density operator has certain properties

- $p^2=p$
- $\rho^\dagger = \rho$
- $Tr(p)=1$
- $p>0$

Justification for Density Matrices

- A density matrix is able to describe *mixed states*
    - It does this through linear combinations of pure states
- It is not known whether or not the universe is in a pure state, so to be fully general, a theory must include general descriptions of mixed states.

A simple example

An example of pure states and a density matrix that we learn early is that of polarized light.

- x-polarized light is in a pure state, with a density matrix of p= $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$
- y-polarized light is a different pure state, with a matrix of p= $\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

Some light is in a mixture of half x-polarization and half y-polarization, and has a mixed density matrix of p= $\begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}$

Useful Properties of the Density Matrix

- $dp/dt = -i(Hp-pH)$
    - This is found by letting the wavefunction vary in time and plugging it into the equation
- For an observable A, when trying to measure A
    - $\langle A \rangle = Tr(pA)$ for mixed states

Entropy can be found from density matrices!

- For a system with density matrix p:
- $S = -Tr(p \ln(p))$

Density Matrices in Statistical Mechanics

Say we have a system with eigenvector $|\psi>$ and corresponding eigenvalue E_i, with Hamiltonian H.

- The density matrix is the sum of $w_n\ |\psi_n><\psi_n|$, where w_n $=1/Q\ (e^{-\beta En})$
- This can be written as $p=e^{-H/kT}/Tr(e^{-H\beta})$
- This means we can find the average energy, which is U=Tr(pH)

More Stat Mech

- From the equation F=U-TS, we can plug in to find
  - $F \leq F_0 + Tr[(H-H_0)e^{-H0/kT}]/Tr[e^{-H0/kT}]$, where H_0 is any other Hamiltonian and F_0 is the corresponding free energy
- By considering the density matrix as a function of β, it can be shown that $-dp/d\beta = Hp$
  - A use of this is in position representation
  - $-dp(xx';\beta)/d\beta = H_x p(xx';\beta)$

Example: Free Particle

- Hamiltonian of a free particle: $H=\boldsymbol{p}^2/2m$
- Equation becomes $-dp(x,x',\beta)/d\beta=-\hbar^2/2m *d^2/dx^2\ p(x,x',\beta)$
- This has the solution $p=sqrt(m/2\pi\hbar^2\beta)\ e^{-(m/2\hbar\text{^}2\beta)(x-x')\text{^}2}$
- For a system of length L, the trace of this equation equals
  - $e^{-\beta F}=L\ sqrt(mkT/2\pi\hbar^2)$
  - Partition function

Example 2: Simple Harmonic Oscillator

- For a linear harmonic oscillator, $H=\boldsymbol{p}^2/2m+mw^2x^2/2$
- $-dp/d\beta=-\hbar^2/2m * d^2/dx^2p + mw^2x^2p/2$
- We can define $a = \text{sqrt}(mw/\hbar)x$ and $f=hw/2$
  - So $-dp/df = -dp^2/da^2+a^2p$
  - This evaluates to approximately $p(a, a', f) = \text{sqrt}\,(mw/4\pi\hbar f)e^{-(a-a')\text{^}2/4f}$
  - To test this, we can try an exponential function, and solve a quadratic equation
- Eventually, we get the final form:
- $p(x,x',\beta)=\text{sqrt}(mw/(2\pi\hbar\ \sinh(hw/kT)))\ *e^{\{-mw/(2h\ \sinh(2f))\ [(x\text{^}2+x'\text{^}2)\ \cosh\ (2f)-2xx']\}}$

References

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