

# Density Matrices

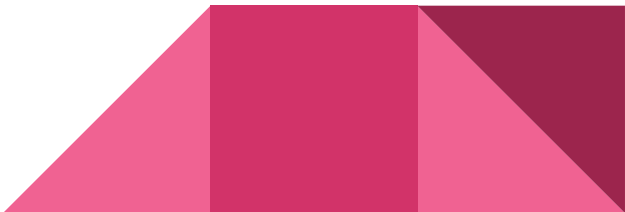
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# Defining a Density Matrix

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

- 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

- $\rho^2 = \rho$
  - $\rho^\dagger = \rho$
  - $\text{Tr}(\rho) = 1$
  - $\rho \geq 0$
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# 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  $\rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$
- y-polarized light is a different pure state, with a matrix of  $\rho = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

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



# 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  $A$ 
  - $\langle A \rangle = \text{Tr}(pA)$  for mixed states

Entropy can be found from density matrices!

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



# Density Matrices in Statistical Mechanics

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

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



# More Stat Mech

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



# Example: Free Particle

- Hamiltonian of a free particle:  $H = \mathbf{p}^2/2m$
- Equation becomes  $-dp(x,x',\beta)/d\beta = -\hbar^2/2m * d^2/dx^2 p(x,x',\beta)$
- This has the solution  $p = \sqrt{m/2\pi\hbar^2\beta} e^{-(m/2\hbar^2\beta)(x-x')^2}$
- 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,  $H = p^2/2m + mw^2x^2/2$
- $-dp/d\beta = -\hbar^2/2m * d^2/dx^2p + mw^2x^2p/2$
- We can define  $a = \sqrt{mw/\hbar}x$  and  $f = \hbar w/2$ 
  - So  $-dp/df = -dp^2/da^2 + a^2p$
  - This evaluates to approximately  $p(a, a', f) = \sqrt{mw/4\pi\hbar f} e^{-(a-a')^2/4f}$
  - To test this, we can try an exponential function, and solve a quadratic equation
- Eventually, we get the final form:
- $p(x, x', \beta) = \sqrt{mw/(2\pi\hbar \sinh(\hbar w/kT))} * e^{\{-mw/(2\hbar \sinh(2f)) [(x^2 + x'^2) \cosh(2f) - 2xx']\}}$



# References

Bertlmann, Reinhold A. *Anomalies in Quantum Field Theory*. Univ. Pr., 2005.

Feynman, R. P. *Statistical Mechanics: a Set of Lectures*. W.A. Benjamin, 1972.

