Quantum Statistics?

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Outline

1. Density Operator & Density Matrix
2. Quantum Statistics
3. The quantum harmonic oscillator
4. Free particle in finite wall
5. Expectation value

Density Operator (Other ways to formulate quantum theory,)

$$\hat{\rho} \equiv |\Psi\rangle\langle\Psi|.$$

Density Matrix

$$\rho_{ij} = \langle e_i \mid \hat{\rho} \mid e_j \rangle = \langle e_i | \Psi \rangle \langle \Psi \mid e_j \rangle$$

For example, an electron with spin up along the x direction

$$|\Psi\rangle = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

$$\rho = |\Psi\rangle\langle\Psi| = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

Projection operator => $\hat{P}_{\Psi} = |\Psi\rangle \langle\Psi|$

Good properties for mixed state

$$|\Psi\rangle = \sum_k c_k |\Psi_k\rangle$$

$$\hat{\rho} = |\Psi\rangle \langle\Psi| = \sum_k p_k |\Psi_k\rangle \langle\Psi_k| , \quad |c_k|^2 = p_k$$

Do not confuse a linear combination of two pure states, which itself is still a pure state. A mixed state, which is not represented by any (single) vector. We just don't know the state of the particles.

Good properties for mixed state. I’m wrong.

$$\cancel{\left|\Psi\right\rangle = \sum_k c_k \left|\Psi_k\right\rangle}$$

$$\hat{\rho} = \left|\Psi\right\rangle\left\langle\Psi\right| = \sum_k p_k \left|\Psi_k\right\rangle\left\langle\Psi_k\right|, \quad \cancel{\left|c_k\right|^2 = p_k}$$

An electron with spin up along x is not mixed state !

Correct and Good properties

$$\hat{\rho} = \sum_k p_k \left|\Psi_k\right\rangle \left\langle\Psi_k\right| = \sum_k p_k \hat{\rho}_k$$

$$\left\langle \hat{A} \right\rangle = \mathrm{Tr}\left(\hat{\rho}\hat{A}\right)$$

The trace won't change under change of basis.

Proof: From this website

Recall that

$$Tr(|\phi_1\rangle\langle\phi_2|) = Tr(|\phi_1\rangle \otimes \langle\phi_2|) = \langle\phi_1 \mid \phi_2\rangle,$$

and

$$\hat{O} \circ (|\phi_1\rangle\langle\phi_2|) = (\hat{O}|\phi_1\rangle) \otimes \langle\phi_2|$$

Now, using the linearity of the trace, we can compute the expectation value as:

$$\langle\hat{O}\rangle = p_1 \langle\psi_1|\hat{O}|\psi_1\rangle + p_2 \langle\psi_2|\hat{O}|\psi_2\rangle$$

$$= p_1 Tr(\hat{O}|\psi_1\rangle\langle\psi_1|) + p_2 Tr(\hat{O}|\psi_2\rangle\langle\psi_2|)$$

$$= Tr(\hat{O}(p_1 |\psi_1\rangle\langle\psi_1|) + p_2 |\psi_2\rangle\langle\psi_2|)) = Tr(\hat{O}\rho)$$

Quantum Statistics(i.e. Quantum State + Boltzmann Distribution)

$$\left\{\begin{array}{c}\text{probability of being}\\ \text{in energy level } n\end{array}\right\} = \frac{1}{Z}\,\mathrm{e}^{-\beta E_n}$$

$$\hat{\rho} = \frac{1}{Z}\sum_n e^{-\beta E_n}\hat{\rho}_n = \frac{1}{Z}\sum_n e^{-\beta E_n}\left|\Psi_n\right\rangle\left\langle\Psi_n\right|$$

The quantum harmonic oscillator (with natural units)

$$H\psi_n^{\text{h.o.}} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2\right)\psi_n^{\text{h.o.}} = E_n\psi_n^{\text{h.o.}}.$$

Recursion method

procedure `harmonic-wavefunction`

input x

$\psi_{-1}^{\text{h.o.}}(x) \leftarrow 0$ (unphysical, starts recursion)

$\psi_0^{\text{h.o.}}(x) \leftarrow \pi^{-1/4}\exp\left(-x^2/2\right)$ (ground state)

for $n = 1, 2, \ldots$ **do**

$\left\{\ \psi_n^{\text{h.o.}}(x) \leftarrow \sqrt{\frac{2}{n}}x\psi_{n-1}^{\text{h.o.}}(x) - \sqrt{\frac{n-1}{n}}\psi_{n-2}^{\text{h.o.}}(x)\right.$

output $\{\psi_0^{\text{h.o.}}(x), \psi_1^{\text{h.o.}}(x), \ldots\}$

The density matrix (It's actually trivial.)

procedure `harmonic-density`

input $\{\psi_0^{\text{h.o.}}(x), \ldots, \psi_N^{\text{h.o.}}(x)\}$ (from Alg. 3.1 (`harmonic-wavefunction`))

input $\{\psi_0^{\text{h.o.}}(x'), \ldots, \psi_N^{\text{h.o.}}(x')\}$

input $\{E_n = n + \frac{1}{2}\}$

$\rho^{\text{h.o.}}(x, x', \beta) \leftarrow 0$

for $n = 0, \ldots, N$ **do**

$\quad \{\ \rho^{\text{h.o.}}(x, x', \beta) \leftarrow \rho^{\text{h.o.}}(x, x', \beta) + \psi_n^{\text{h.o.}}(x)\psi_n^{\text{h.o.}}(x')\mathrm{e}^{-\beta E_n}$

output $\{\rho^{\text{h.o.}}(x, x', \beta)\}$

Why it's trivial in this case.

$$\hat{\rho}_1 = |\Psi_1\rangle \langle\Psi_1| = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

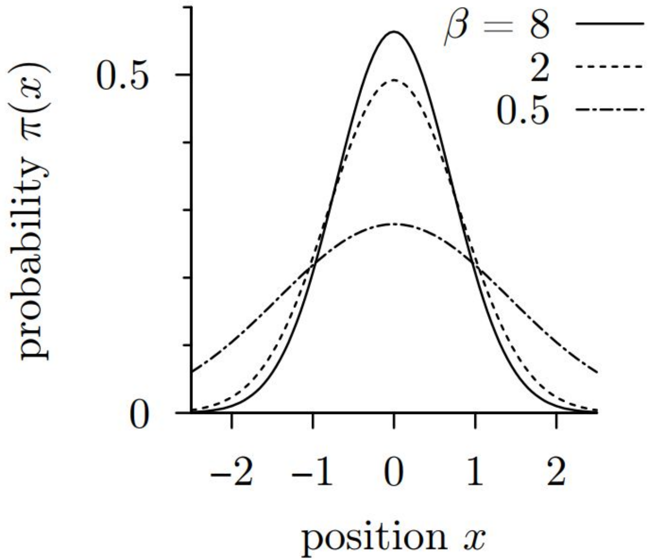
$$\hat{\rho} = \sum_n p_n \hat{\rho}_n = \begin{pmatrix} e^{-\beta E_1} & 0 & 0 \\ 0 & e^{-\beta E_2} & 0 \\ 0 & 0 & e^{-\beta E_3} \end{pmatrix}$$

Probability to be at position x

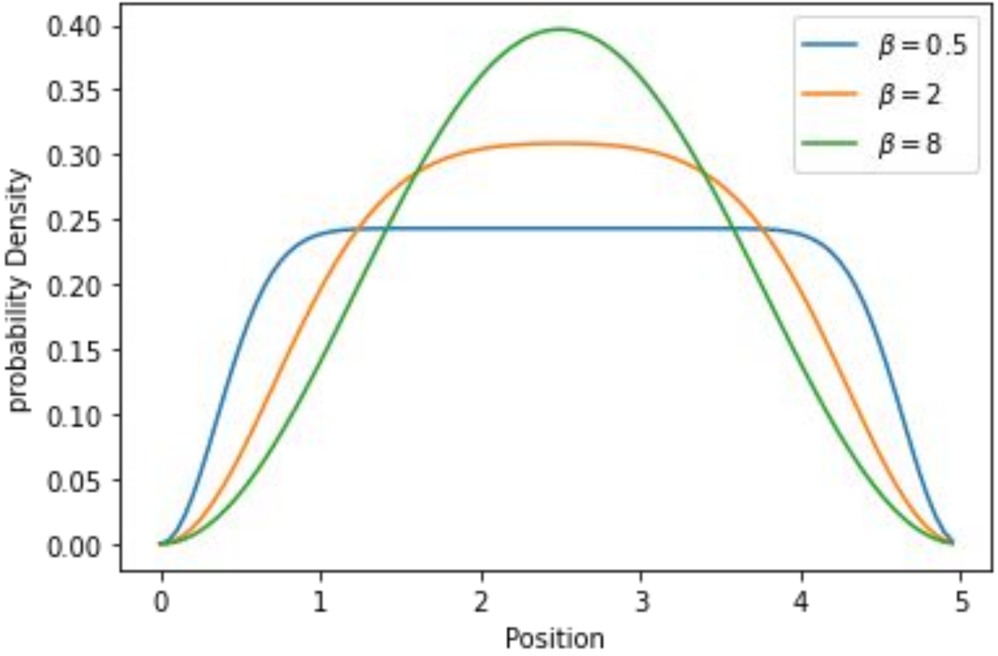
$$\pi(x) = \left\{ \begin{matrix} \text{probability of being} \\ \text{at position } x \end{matrix} \right\} \propto \rho(x, x, \beta) = \sum_n \mathrm{e}^{-\beta E_n} \psi_n(x) \psi_n^*(x)$$

Note:

$$\beta \propto \frac{1}{T}$$



Another example is a free particle in a box of hard walls. With the almost the same code.



Expectation value！

I have mentioned that

$$\langle \hat{A} \rangle = \mathrm{Tr}\left(\hat{\rho}\hat{A}\right)$$

Here are the implements. I will calculate for
1. Twice_momentum_operator
2. Momentum Operator
3. Position Operator

With the configuration of free particle in box of hard walls.

The density matrix is easy just like before

$$\hat{\rho}_1 = |\Psi_1\rangle \langle\Psi_1| = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\hat{\rho} = \sum_n p_n \hat{\rho}_n = \begin{pmatrix} e^{-\beta E_1} & 0 & 0 \\ 0 & e^{-\beta E_2} & 0 \\ 0 & 0 & e^{-\beta E_3} \end{pmatrix}$$

The idea of finding the matrix of operator

$$|\Psi\rangle = \sum_n c_n |\Psi_n\rangle \quad \hat{O}|\Psi\rangle = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

Find: $\hat{O}\phi_n = \sum_m a_{mn}\phi_m$

Twice Momentum Operator

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

$$\hat{p}^2 \phi_n = \left(\frac{n\pi}{L}\right)^2 \phi_n$$

```python
def twice_momentum_operator(N,L):
    tmp = np.zeros(shape=(N,N))
    for n in range(1,N+1):
        tmp[n-1][n-1] = pow(n*np.pi/L,2)
    return tmp
```

Momentum Operator

$$\hat{p}\phi_n = -i\sqrt{\frac{2}{L}}\frac{n\pi}{L}\cos\frac{n\pi}{L}x = \sum_m a_{mn}\phi_m$$

Use Fourier trick to get the coefficients.

$$\langle \hat{\rho}\phi_n | \phi_k \rangle = a_{kn}$$

Code explanation

```python
def fourier_trick_cos(n,M,L):        # cos(nx) & sin(mx)
    coefficients = np.zeros(M+1, dtype='complex_')
    for m in range(1,M+1):
        func = lambda x: (2/L)*(n*np.pi/L)*np.cos(n*np.pi*x/L)*np.sin(m*np.pi*x/L)
        result = -1*integrate.quad(func, 0, L)[0]
        if abs(result) < 10E-9:
            result = 0
        coefficients[m] = complex(0, result)
    return coefficients
```

Put numbers in

```python
def momentum_operator(N,L):
    tmp = np.zeros(shape=(N,N), dtype='complex_')
    for n in range(1,N+1):
        vec = fourier_trick_cos(n,N,L)
        for m in range(1,N+1):
            tmp[m-1][n-1] = vec[m]
    return tmp
```

$$x\phi_n = \sum_m a_{mn}\phi_m$$

```python
def fourier_trick_x(n,M,L):        # x & sin(nx)
    coefficients = np.zeros(M+1)
    for m in range(1,M+1):
        func = lambda x: x*(2/L)*np.sin((n*np.pi*x)/L)*np.sin((m*np.pi*x)/L)
        result = integrate.quad(func, 0, L)[0]
        coefficients[m] = result
    return coefficients
```

The results of numerical methods and Analytic solution

```
trace_two_matrix(density_matrix(10,5,2), twice_momentum_operator(10,5))
trace_two_matrix(density_matrix(10,5,2), momentum_operator(10,5))
trace_two_matrix(density_matrix(10,5,2), position_operator(10,5))
```

✓ 0.5s

```
0.7745822618806789
0
2.5
```

$$\langle p^2 \rangle = \sum_n p_n \left(\frac{n\pi}{L}\right)^2 = 0.7745822618806789$$

$$\langle p \rangle = \frac{d}{dt} x = 0$$

$$\langle x \rangle = \frac{L}{2} = 2.5$$

Questions

Reference

1. Werner Krauth - Statistical Mechanics_ Algorithms and Computation 3.1
2. Introduction to Quantum Mechanics (David J. Griffiths, Darrell F. Schroeter) Chap 2, 3, 12.3.
3. quantum mechanics - What is the actual meaning of the density operator? - Physics Stack Exchange
4. https://www.youtube.com/watch?v=bg0SMY40q8Q&ab_channel=ProfessorMdoesScience
5. https://www.youtube.com/watch?v=DQEtg8pWT8E&ab_channel=ProfessorMdoesScience

Modules

1. Numpy
2. Matplotlib
3. Scipy