

“Measuring” the Density Matrix

Introduction

Schrödinger's quantum mechanics and its statistical postulates are usually formulated in terms of a state (wave) function, $|\Psi\rangle$ which is a solution to Schrödinger's equation. Alternatively, these statistical postulates can be formulated in terms of a *density operator* ρ_{op} , which is defined as

$$\rho_{op} = |\Psi\rangle\langle\Psi|, \quad (1)$$

a choice which, in many ways, is more general and useful than the state (wave) function formulation. For one thing, the density operator is a *measurable*. i.e. it is determined by observables, whereas the state (wave) function is *not*. (There is, in fact, no way to determine a wave function by measurements.) This alone is certainly a good incentive. Another practical reason for choosing the density operator formulation is that it is capable of accommodating a broader description of quantum “states” – in particular “states” which are not “*pure*”, i.e. “states” for which “information” content is ***less than 1***. This is a major stride towards defining thermodynamics. For pure state density operators [see Eq.1] possess *complete knowledge* of the quantum system, whereas thermodynamic systems are those about which *knowledge is incomplete*. There is *no* state function that describes *that* practical (thermal) condition.

On the other hand, there *is* a quantum object – called the *Mixed State Density operator* – that does accommodate incomplete knowledge and within which lies the quantum basis of thermodynamics.

Therefore, to extend the reach of quantum mechanics to thermal situations the density operator concept is a crucial bit of quantum mechanics that must be brought to our attention. One can, indeed, shed the state vector $|\Psi\rangle$ habit formed by introductory “QM” pedagogy and everywhere replace it by the density operator of Eq.1.

In this lab we focus on the density operator, especially its corresponding matrix as generated by a particular choice of expansion basis.

Objectives

Unlike a wave function which is NOT a measurable, the density operator (matrix) is, in principle, determined by measurables. The issue of “measuring” a density matrix reduces largely to how many distinct measurements are necessary and which ones.

SPINS is a computer simulation that conducts a variety of computer experiments involving randomly polarized spin-1/2 atoms emanating from, say, an oven.

1. We use the simulated Stern-Gerlach apparatus to find the density matrix corresponding to each of the program’s modeled sources.
2. We will use two different definitions of information to calculate the information content associated with each of these density matrices.
3. We will decide if each density matrix represents a pure or mixed state.

Theory I

If a system can exist in N linearly independent quantum states, say $|\phi_i\rangle$, $i = 0, 1, \dots, N$, the density matrix

$$\rho_{m,n} = \langle \phi_m | \rho_{op} | \phi_n \rangle = \langle \phi_m | \Psi \rangle \langle \Psi | \phi_n \rangle \quad (2)$$

will have N rows and N columns. Since a density matrix has the property $Tr \rho_{op} = 1$, it has $N^2 - 1$ independent elements. (A spin 1/2 system can exist in two states, usually taken as states quantized parallel and anti-parallel to a z -axis, so that the density matrix is of dimension 2×2 and has 3 independent elements.) Assume now that we can find N^2 linearly independent $N \times N$ hermitian operators Ω_s ,

$$\Omega = \{\Omega_1, \Omega_2, \Omega_3 \dots, \Omega_{N^2}\} \quad (3)$$

that are “orthogonal” in the sense that

$$Tr \Omega_j \Omega_k = \delta_{jk} \quad (4)$$

[**Note:** Finding such “orthogonal” operators may, in general, be much easier said than done. But for this exercise there is no difficulty. See R. G. Newton and B.

Young, *Annals of Physics* **49**, 393 (1968).] We can then expand any $N \times N$ observable Γ as

$$\Gamma = \sum_{s=1}^{N^2} \gamma_s \Omega_s \quad (5)$$

where the coefficients are

$$\gamma_s = Tr \Gamma \Omega_s. \quad (6)$$

We are interested in the particular case $\Gamma \equiv \rho_{op}$ (a density operator) so that Eq. 5 becomes

$$\rho_{op} = \sum_{s=1}^{N^2} \rho_s \Omega_s \quad (7)$$

whose expansion coefficients are

$$\rho_s = Tr \rho_{op} \Omega_s \quad (8)$$

$$= \langle \Omega_s \rangle \quad (9)$$

where $\langle \Omega_s \rangle$ is the average value of Ω_s . The density operator (matrix) is, therefore, totally characterized by the “complete set” of average values $\langle \Omega_s \rangle$, i.e.,

$$\rho = \sum_{s=1}^{N^2} \langle \Omega_s \rangle \Omega_s \quad (10)$$

or in terms of matrix elements

$$\langle m | \rho | n \rangle = \sum_{s=1}^{N^2} \langle \Omega_s \rangle \langle m | \Omega_s | n \rangle. \quad (11)$$

Theory II

The average value of any observable Γ is expressible in terms of the density operator ρ_{op} as

$$\langle \Gamma \rangle = Tr \rho_{op} \Gamma \quad (12)$$

$$= \sum_{s=1}^{N^2} \gamma_s Tr \rho_{op} \Omega_s \quad (13)$$

$$= \sum_{s=1}^{N^2} \gamma_s \langle \Omega_s \rangle \quad (14)$$

where Eq.5 has been used to obtain Eq. 13.

If the “orthogonal” expansion matrices $\langle m|\Omega_s|n\rangle$ are *traceless*, then the *identity matrix* $\Omega_0 = \nu\mathbf{I}$, where ν is a normalizing factor, can be included as a basis member, which means that only $N^2 - 1$ *non-trivial* basis matrices are required.

The proof of this follows from the orthogonality condition Eq. 4. For assume that $\Omega_0, \Omega_1, \Omega_2, \dots, \Omega_s$ form a basis such that $\Omega_1, \Omega_2, \dots, \Omega_s$ are traceless, i.e.

$$Tr \Omega_k = \sum_m \langle m|\Omega_k|m\rangle = 0; k \neq 0. \quad (15)$$

Then with $\Omega_0 = \nu\mathbf{I}$ as the remaining member of the basis we can still write

$$Tr \Omega_0 \Omega_k = 0; k \neq 0 \quad (16)$$

which satisfies the orthogonality requirement. Thereby Ω_0 completes the basis.

But Ω_0 must still be normalized, i.e.

$$Tr \Omega_0 \Omega_0 = \nu^2 Tr \mathbf{I} = 1 \quad (17)$$

which requires

$$\Omega_0 = \frac{\mathbf{I}}{\sqrt{Tr \mathbf{I}}} \quad (18)$$

in which case from Eqs. 7 and 8 the coefficient

$$\rho_0 = \langle \Omega_0 \rangle = Tr \rho_{op} \Omega_0 \quad (19)$$

$$= Tr \rho_{op} \frac{\mathbf{I}}{\sqrt{Tr \mathbf{I}}} \quad (20)$$

$$= \frac{1}{\sqrt{Tr \mathbf{I}}} \quad (21)$$

where

$$Tr \rho_{op} \mathbf{I} = 1. \quad (22)$$

Example: Spin 1/2

A spin 1/2 system (ignoring all degrees of freedom other than spin) can be constructed using a basis of the two spin S_z eigenstates $|1/2\rangle$ and $|-1/2\rangle$ where

$$S_z |\pm 1/2\rangle = \pm \frac{\hbar}{2} |\pm 1/2\rangle. \quad (23)$$

Thus, the density matrix for spin 1/2 is only 2×2 and consists of the 4 independent elements,

$$\rho = \begin{pmatrix} \langle 1/2 | \rho_{op} | 1/2 \rangle & \langle 1/2 | \rho_{op} | -1/2 \rangle \\ \langle -1/2 | \rho_{op} | 1/2 \rangle & \langle -1/2 | \rho_{op} | -1/2 \rangle \end{pmatrix} \quad (24)$$

An orthogonal basis, in the sense of Eq. 4, is quite naturally the matrices,

$$\Omega_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \Omega_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \Omega_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (25)$$

where

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (26)$$

are the 3 Pauli spin matrices [Matrices of angular momentum operators S_j in the basis $|1/2\rangle$ and $|-1/2\rangle$, as defined in Eq. 23, are $S_j = \frac{\hbar}{2}\sigma_j$.] Furthermore, the matrices of Eqs. 25 all have zero trace, so that a trivial *unit matrix* (properly normalized)

$$\Omega_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (27)$$

can be added to the basis giving the required $N^2 = 4$ basis matrices. Then using the expansion in Eq. 10 we have

$$\rho = \rho_0 + \sum_{j=1}^3 \langle \Omega_j \rangle \Omega_j \quad (28)$$

$$= \left[\frac{\mathbf{I}}{2} + \frac{1}{\hbar} (\langle S_x \rangle \sigma_x + \langle S_y \rangle \sigma_y + \langle S_z \rangle \sigma_z) \right]. \quad (29)$$

By measuring the observables $\langle S_x \rangle, \langle S_y \rangle, \langle S_z \rangle$ we can construct a spin 1/2 density matrix.

For higher values of angular momentum the problem becomes more complex but the density matrix reconstruction is still possible.

The Experiment

1. Prepare the computer simulation by double clicking on the .jar file called “spins.
Read the accompanying “Notes for SPINS program.
2. Reset all the counters.

3. Choose the first source option by selecting its radio button.
4. Choose the field gradient orientation \mathbf{x} .
5. Start the flow of particles from the oven.
6. After a few hundred particles have registered in the detectors stop the particle flow.
7. Determine the *average value* of spin component S_x .
8. Reset counters and repeat for S_y and then for S_z .

The Analysis

1. Use Eqs. 26 and 29 to construct the density matrix for each source.
2. Calculate the “*Information*” \mathcal{I} for each density matrix,

$$\mathcal{I} = \text{Tr} \rho^2 \tag{30}$$

3. Calculate the “*Missing Information*” \mathcal{S} for each density matrix,

$$\mathcal{S} = -\text{Tr} \rho \ln \rho. \tag{31}$$

[How will you calculate \mathcal{S} ?]

4. Based on the results in 2. and 3. determine which sources are pure and which are mixed.
5. Discuss what is meant by pure vs. mixed in terms of thermodynamic content.