

Density Matrix Formalism

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In this paper, we attempt to provide an introductory description of quantum mechanics formulated in terms of the density matrix. Although entirely equivalent to the commonly encountered state vector for deterministic quantum systems, the density matrix encompasses a more general class of systems where "less than maximum information" is known about the initial preparation of the system. Our focus will be primarily to elucidate the abstract notions associated with this formalism while keeping the mathematical constructs to a minimum.

I. INTRODUCTION

Ascertaining the maximum amount of information about a given physical system is one of the primary drives behind scientific pursuit. Unfortunately, assigning a completely deterministic state to a system where all of its parameters are known is not only an impractical task, but it is inherently impossible. To what degree of missing information then is a system's properties and evolution still adequately described? Classically, this question was addressed and answered using statistical mechanics: as opposed to examining the evolution of each individual micro-state, statistical ensembles corresponding to a given macro-state provided accurate thermodynamic properties of the system when maintained at equilibrium. Without knowing the exact location of all $\approx 10^{23}$ molecules, extremely precise properties of a system can be measured.

The success of classical statistical mechanics defined it as one of the cornerstones of science; however, the analysis remains classical and a full quantum description of the system's state is unaccounted for. In contrast to classical physics, it is conventional to represent the quantum state of a system by its state vector $|\Psi\rangle$ which evolves in time according to the Schrödinger equation given the initial state is precisely known. Often though, we don't know the exact state vector of the system. For example, photons from a thermal source do not have a precise polarization and so the system could not be completely described in terms of a single state vector. This is precisely what defines the difference between a *pure* and a *mixed* state and is the motivation behind the density matrix formalism.

II. PURE VERSUS MIXED STATES

Consider, as above, a beam of photons emitted from a thermal source. As a simple experiment to characterize the state of the beam, imagine placing a polarizer which can rotate about the optical path. Now consider the exact same setup, except replace the source of the photons

with a laser having a well defined polarization oriented at 45 degrees with respect to the polarizer. Quantum mechanically, we could write the state of the laser's photons as a vector $|\Psi\rangle = \frac{1}{\sqrt{2}}(|e_x\rangle + |e_y\rangle)$, where $|e_{x,y}\rangle$ are the orthonormal x/y-axis. States with the maximum information, such as this one, are referred to as "pure" states. From our interpretation of quantum mechanics, we would then claim that there is a 50% chance of a photon passing through the polarizer. Thus, we would expect the intensity to drop by half after passing through, which, is indeed what happens. On the other hand, if we pass the beam of photons generated from the thermal source we would also observe a decrease in intensity by half irrespective of the angle of the polarizer. It then follows that it is impossible to write the state of the thermal photons in any form of $|\Psi\rangle = \alpha|e_x\rangle + \beta|e_y\rangle$, otherwise the polarization of the thermal photons could be measured. However, it is possible to describe the state of the thermal photons in a probabilistic fashion. Since half of the photons always pass through the polarizer, no matter the angle, it is reasonable to say that each photon is either in the state $|e_x\rangle$ with a 50% probability or $|e_y\rangle$ with 50% probability. Thus, the state of the unpolarized light can be described as a statistical ensemble of quantum pure states; this is what is referred to as a "mixed" state. We can formally write the vector of a mixed state by specifying a set of pure state $\{|\Psi^{(n)}\rangle\}$ and the associated classical probabilities $\{p^{(n)}\}$. The mixed state is then given by

$$|\Psi_{mixed}\rangle = p^{(1)}|\Psi^{(1)}\rangle + p^{(2)}|\Psi^{(2)}\rangle + \dots + p^{(n)}|\Psi^{(n)}\rangle. \quad (1)$$

The distinction between mixed and pure states can be subtle. It must be stressed that a mixed state is not a superposition of pure states. Pure states are characterized by the existence of some observable which is consistently measured when performed on that state and in that state only. When the information is less than maximum (polarization of the thermal photons) the state is considered mixed. It is also worth noting that the basis representation of a mixed state is not unique; the choice of linear polarization vectors could have easily been replaced with the orthogonal circular polarization basis.

Mixed states arise in many scenarios, particularly in the preparation step of an experiment. Since experiments are repeated multiple times, the entire set of experiments may be thought of as an ensemble of known pure state. It is a realistic expectation that many of these were not pre-

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pared in exactly the same state, thus there is some probability that the experiment will measure several different pure states. Additionally, a single experiment could be performed on a collection of state, all of which may not be in the same state. A final example of when one might encounter a mixed state is in the case of a coupled system. For instance, consider a system which is coupled to a reservoir. Globally, we could construct the entire system+reservoir state function, but this is cumbersome since we do not really care about how the reservoir behaves. So, instead of specifying precisely the wave function of the entire system, we assign a set of probabilities each corresponding to a possible pure states; the result is exactly a mixed state. It can be gleamed from this analysis that the set of probabilities is closely related to the probability distributions in statistical mechanics. Indeed, there is an almost one-to-one correspondence. Later, as an example, we will find that the density matrix can be thought of as the quantum mechanical counterpart of the probability distribution of statistical mechanics and that its form is nearly identical.

III. THE DENSITY MATRIX

A. Formulation

Motivated by the prior discussion, it is reasonable to suspect that the ordinary formalism of quantum mechanics may not accurately incorporate, or, at least, may not be well suited to handle the concept of mixed states. Consider a pure quantum state $|\Psi\rangle$ identified by the coefficients c_i in it's complete expansion into eigenvectors $|u_i\rangle$ of some set of commuting observables, i.e.

$$|\Psi\rangle = \sum_i c_i |u_i\rangle. \quad (2)$$

Given an operator \hat{O} , the mean value is then calculated according the operators corresponding matrix O_{ij} ,

$$\langle\hat{O}\rangle = \sum_{i,j} c_i^* c_j \langle u_i | \hat{O} | u_j \rangle = \sum_{i,j} c_i^* c_j O_{ij}. \quad (3)$$

For the case of a mixed state, the expansion of the wave function is over a set of pure states $\{|\Psi^{(n)}\rangle\}$ each with statistical weight $\{p^{(n)}\}$ (see equation 1). The mean value of an operator \hat{O} is then given by the average of mean values associated with each pure state,

$$\langle\hat{O}\rangle = \sum_n p^{(n)} \langle O \rangle_n = \sum_{i,j} O_{ji} \sum_n p^{(n)} c_j^{(n)*} c_i^{(n)}. \quad (4)$$

If we define the matrix,

$$\rho_{ij} = \sum_n p^{(n)} c_j^{(n)*} c_i^{(n)}, \quad (5)$$

then (4) becomes,

$$\langle\hat{O}\rangle = \sum_{i,j} O_{ji} \rho_{ij} = Tr(O\rho), \quad (6)$$

where $Tr()$ indicates the trace of a matrix.

We have shown that the corresponding state of a system, albeit mixed or pure, may be defined in terms of a matrix (5) and that the expectation value of a given operator is given by (6). This matrix is called the *Density Matrix* and carries with it precisely the same information as if the state vector had been specified. It represents the minimum set of information required to calculate the mean value of an operator and is constructed using the knowledge of the state prior to measurement. In the next section, we briefly highlight several important features of the density operator.

B. Basic Properties

Given the density matrix ρ_{ij} the following features hold:

(1) Given a Hermitian operator \hat{O} , the condition that $\langle O \rangle$ be real implies ρ is also Hermitian:

$$\rho_{ij} = \rho_{ji}^*. \quad (7)$$

(2) ρ is *positive definite*. That is to say, every diagonal element is always greater or equal to zero,

$$\rho_{ii} \geq 0. \quad (8)$$

(3) The trace of ρ^2 is always less than or equal to 1,

$$Tr(\rho^2) \leq 1. \quad (9)$$

Additionally $Tr(\rho^2) = 1$ if and only if the state is pure. This can sometime serve as a definition between a mixed and pure state

(4) The temporal evolution of the density matrix is governed by the *Liouville-von Neumann equation*,

$$i\hbar \frac{\partial \rho}{\partial t} = [H, \rho], \quad (10)$$

which follows directly from the Shrodinger equation when the state is taken in the Shrodinger picture. If the Hamiltonian H is time-independent, (10) may be directly integrated to yield,

$$\rho(t) = e^{-iH(t-t_o)/\hbar} \rho(t_o) e^{iH(t-t_o)/\hbar}. \quad (11)$$

IV. EXAMPLES

A. Thermal Equilibrium

Consider a system in thermal equilibrium at temperature T and governed by Hamiltonian H . The various quantum pure states will thus form a distribution over the various states compatible with the total energy of the system. We already know that the probability is determined by the canonical distribution, so we may write

the associated density matrix as

$$\rho(T) = \sum_{k=1}^{\infty} p(E_k) |k\rangle \langle k| = \frac{1}{Z} \sum_{k=1}^{\infty} e^{-E_k/kT} |k\rangle \langle k| \quad (12)$$

where Z is the partition function $\sum_{k=1}^{\infty} e^{-E_k/kT}$ and the set of pure states $\{|k\rangle\}$ are energy eigenvectors of the Hamiltonian. Thus the density matrix is in exactly the same form as the distribution function from classical statistical mechanics.

B. Two-level system: Optical Bloch Equations without decay

For an atom driven by an oscillating electric field near resonance, it is well justified to reduce the system to a two dimensional Hilbert space consisting of a ground $|g\rangle$ and excited state $|e\rangle$. By assuming that the state of the atom is pure, we can write the wave function as,

$$|\Psi\rangle = C_e |e\rangle + C_g |g\rangle. \quad (13)$$

By neglecting higher order moments, the interacting portion of the Hamiltonian due to the monochromatic electric field perturbation is given by,

$$H_I = -\frac{e\langle x\rangle E_o}{2}(e^{i\omega t} + e^{-i\omega t}) \quad (14)$$

where $\langle x\rangle$ is the expectation value of the position operator. The wave function then satisfies the Shrodinger Equation,

$$i\hbar \frac{\partial |\Psi\rangle}{\partial t} = (H_o + H_I) |\Psi\rangle \quad (15)$$

which, after substitution of (13) and (14), yields two coupled first-order differential equations for the coefficients. In accordance with the definition of the density matrix, this set of equations may be transformed into a set of three equations for the density matrix elements. The fi-

nal result is,

$$\frac{d\rho_{ee}}{dt} = \frac{i\Omega}{2}(e^{-i\omega t}\rho_{eg} - e^{i\omega t}\rho_{ge}) \quad (16a)$$

$$\frac{d\rho_{gg}}{dt} = -\frac{i\Omega}{2}(e^{-i\omega t}\rho_{eg} - e^{i\omega t}\rho_{ge}) \quad (16b)$$

$$\frac{d\rho_{eg}}{dt} = -i\omega_{eg}\rho_{eg} + \frac{i\Omega}{2}e^{-i\omega t}(\rho_{eg} - \rho_{ge}) \quad (16c)$$

where $\Omega = e\langle x\rangle E_o/\hbar$. The final element of the density matrix follows from the hermitian condition, i.e. $\rho_{eg} = \rho_{ge}^*$. This set of equations is known as the Bloch Equations and are of great importance to the study of light-matter interactions.

V. CONCLUSION

We have shown an entirely equivalent formulation of the description of quantum systems through the use of the density matrix. Although there is no loss of generality when considering state vectors, the density matrix is a more natural way to address systems with less than maximum information regarding the system's initial preparation. The basic properties and several examples were discussed. It should be noted that this was a very basic introduction to this entire field of analysis and that there are a multitude of additional details and examples of the density matrix. Particularly, the interested reader is encouraged to pursue what is known as *Quantized Reservoir Theory* in which subsystems are described through a reduced density matrix and several very important topics, such as the incorporation of damping terms, are investigated.

VI. REFERENCES

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