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Determination of the Quantum State by Measurements*

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A question raised by Pauli as to whether or not the probability densities in space and momentum determine the wave function is answered negatively. The assertion by Kemble that the probability density and its time derivative determine the wave function is shown to be not generally true. It is shown that measurement of the probability density and the probability current determine the wave function of a spinless particle. The measurement of the probability current is discussed. Measurements which determine the spin state and the density matrix of a mixture are also considered.

I. INTRODUCTION

In this paper we are concerned with what measurements may be made on an ensemble of systems representing the same quantum state, to determine that state. In the first two sections, we consider the case in which the system is in a pure quantum state, and in the third section we consider mixtures.

This is a matter of some interest, yet we have found very little discussion of it in the literature. Pauli, in his famous *Handbuch* article,[1] says that it remains an open question (this still appears in the reprinted version) whether or not the distribution function in $\mathbf{r}$, $\rho(\mathbf{r})=|\psi(\mathbf{r})|^2$, and the distribution function in momentum, $\rho(\mathbf{p})=|\int\psi(\mathbf{r})\times\exp(-i\mathbf{p}\cdot\mathbf{r})d\mathbf{r}|^2$, serve to determine $\psi(\mathbf{r})$.[2] That $\rho(\mathbf{r})$ and $\rho(\mathbf{p})$ do *not* determine ψ generally is easily seen. For example, if we take

$$\psi(\mathbf{r})=f(\mathbf{r})P_l{}^m(\theta)e^{im\phi}, \tag{1}$$

$\rho(\mathbf{r})$ and $\rho(\mathbf{p})$ are obviously independent of the sign of m.

Kemble, in his well-known text book,[3] considers this problem, but he errs in extending considerations of Feenberg on one-dimensional motion to higher dimensions. He makes the statement[3] that $\rho(\mathbf{r})$ and $\dot\rho(\mathbf{r})$ are sufficient to determine ψ. That this statement is not generally true is also clear from the example (1), because, if $f(\mathbf{r})$ is real, $\dot\rho(\mathbf{r})=0$ and $\rho(\mathbf{r})$ is independent of the sign of m.

It is immediately apparent that in order to determine ψ it is sufficient to determine the probability density $\rho(\mathbf{r})$ and the probability current $\mathbf{j}(\mathbf{r})$ by measurements carried out on the ensemble of systems in the same pure state. If we write

$$\psi(\mathbf{r})=f(\mathbf{r})\exp[iS(\mathbf{r})\hbar^{-1}], \tag{2}$$

where f and S are real, then

$$\rho(\mathbf{r})=|\psi(\mathbf{r})|\psi(\mathbf{r})|^2=f^2(\mathbf{r}) \tag{3}$$

and

$$\mathbf{j}(\mathbf{r})=(\hbar/2mi)(\bar\psi\nabla\psi-\psi\nabla\bar\psi)=\rho(\mathbf{r})\nabla S(\mathbf{r})m^{-1}. \tag{4}$$

Equations (2)–(4) serve to determine ψ (to within a constant phase) if ρ and $\mathbf{j}$ are determined by measurements.[4]

Although the Born relation [Eq. (3)] is fundamental for the physical interpretation of the mathematical formalism of quantum mechanics, the measurements required to determine the probability current have received relatively little discussion. A *gedanken* experiment to determine $\mathbf{j}(\mathbf{r})$ by measuring the average velocity of the particle at a point, $\langle\mathbf{v}(\mathbf{r})\rangle=\nabla S(r)/m$, is discussed in Appendix A.

There is no difficulty in principle in extending this method for determining ψ to a system containing several particles: one determines $\rho(\mathbf{r}_1,\cdots,\mathbf{r}_n)$ and $\mathbf{j}_i(\mathbf{r}_1,\cdots,\mathbf{r}_n)=\rho(\mathbf{r}_1,\cdots,\mathbf{r}_n)\langle\mathbf{v}_i\rangle=\rho(\mathbf{r}_1\cdots\mathbf{r}_n)\nabla_{\mathbf{r}_i}S(\mathbf{r}_1\cdots\mathbf{r}_n)/m_i$.

II. SPIN STATE

In the preceding section, we neglected spin. If the particle has spin and if the spin state depends upon $\mathbf{r}$ then the analysis of that section becomes somewhat more complicated, but in an uninteresting way. It is of some interest, however, to give brief consideration to the determination of the spin state when spin-orbit coupling can be neglected. This can be done (in principle) by means of the modifield Stern-Gerlach appa-

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[1] W. Pauli, *Encyclopedia of Physics* (Springer-Verlag, Berlin, 1958), Vol. V, p. 17.

[2] For simplicity, we consider the state of a single particle. All of our considerations are nonrelativistic, and are based on the Copenhagen interpretation of the existence of classically described measuring instruments.

[3] E. C. Kemble, *Fundamental Principles of Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1937), p. 71.

[4] One might be concerned about how to determine the relative signs of f on the two sides of a nodal surface of f^2 when ψ is real, say. The relative sign is negative (if ψ is real), or more generally ψ changes sign when passing through a nodal surface since its normal derivative is continuous and nonzero.

ratus as described in Feynman's lectures,[5] which we call a Feynman filter. We refer the reader to Ref. 5 for detailed explanation. Briefly, the apparatus consists of three Stern-Gerlach magnets in series. The two end ones are identical and of the same polarity, whereas the middle one is twice as long as an end one and of the opposite polarity. A parallel beam of particles entering along the axis of the apparatus is separated into $(2S+1)$ spatially separated beams within the apparatus (S = spin) and will be brought back into an unseparated parallel beam upon leaving the apparatus. The advance in phase along each path in the apparatus is the same, so that, for example, if a particle entering the apparatus is in an eigenstate of an arbitrary component of the spin, it will be in that same spin state upon leaving the apparatus. The apparatus is also provided with gates which may be opened or closed, passing or stopping chosen separated beams within the apparatus.

Let $\mathbf{S}$ be the spin of the particle and let $|\hat{r},m\rangle$ be an eigenstate of the $\hat{r}$ component of the spin with eigenvalue m,

$$\hat{r}\cdot\mathbf{S}|\hat{r},m\rangle=m|\hat{r},m\rangle. \tag{5}$$

An arbitrary spin state may be written

$$|\psi\rangle=\sum_{m=-S}^{S} C_m(\hat{r})|\hat{r},m\rangle, \tag{6}$$

$|\psi\rangle$ is determined only to within a phase factor, of course, and fixing its normalization leaves $2S$ moduli and $2S$ (relative) phases of the C's to be determined by measurement. This determination can be done very simply (in principle) with Feynman filters.

Let the Stern-Gerlach magnets separate the $|\hat{z},m\rangle$ states internally; then closing the gates and counting the particles collected at each gate gives us the $|C_m(\hat{z})|^2$.

To determine the relative phase of $C_m(\hat{z})$ and $C_n(\hat{z})$, say, we close all the gates except those corresponding to $S_z=m$, n. The spin state of the particles passing the filter is then

$$\begin{aligned}|\psi'\rangle&=e^{i\phi}(|\hat{z},m\rangle\langle\hat{z},m|+|\hat{z},n\rangle\langle\hat{z},n|)|\psi\rangle\\&=C_m(\hat{z})|\hat{z},m\rangle+C_n(\hat{z})|\hat{z},n\rangle\end{aligned} \tag{7}$$

except for a normalization factor and a common phase factor. We now analyze the spins of the resulting particles in the x-y plane and determine the relative phase of C_m and C_n. If particles in state (7) are analyzed by a Stern-Gerlach magnet which separates the components of $\mathbf{S}\cdot\hat{r}$, where $\hat{r}$ is in the x-y plane and makes an angle ϕ with the x axis,[6] then with the standard choice of phases[7]

$$\begin{aligned}|\langle\hat{r},p|\psi'\rangle|^2=&|d_{pm}{}^S(\pi/2)C_m(\hat{z})|^2+|d_{pn}{}^S(\pi/2)C_n(\hat{z})|^2\\&+2|C_m(\hat{z})C_n(\hat{z})|d_{pm}{}^Sd_{pn}{}^S\cos[(m-n)\phi+\theta_m-\theta_n],\end{aligned} \tag{8}$$

where θ_m and θ_n are the phases of C_m and C_n and the d's are the rotation matrices.[7] By choosing $(m-n)\phi=0$, $-\frac{1}{2}\pi$, say, we determine $\theta_m-\theta_n$.

Of course, there are many other ways to determine the spin state. It can be shown that it generally is *not* sufficient to determine the distribution functions of S_z, S_x, and S_y [an insufficiency somewhat similar to that of the determination of $\rho(\mathbf{x})$ and $\rho(\mathbf{p})$ for the space part of the wave function]; however, as Fano[8] has pointed out, the determination of the mean values of the nonvanishing multipole components of the spin distribution is sufficient to determine the spin state.

III. MIXTURES

In the preceding sections, we supposed that we had a system in a pure quantum state, and we discussed means of determining this state by measurements carried out on an ensemble of systems all in this state. A concrete ensemble generally does not consist of systems all in the same quantum state; it is a mixture, and the state of the ensemble is represented by a density matrix.[9] We discuss measurements on the ensemble which may serve to determine the state of the mixture, first for the spin, then for the cm motion.

Spin. The density matrix for the spins may be written

$$\rho=\sum_{n,m}\rho_{nm}|\hat{z},n\rangle\langle\hat{z},m| \tag{9}$$

in terms of the eigenstates of $\mathbf{S}\cdot\hat{z}$, Eq. (5), where the matrix ρ_{nm} is Hermitian, has positive eigenvalues, and has unit trace.[9] The sums in (9) run from $-S$ to S. For a pure state $\rho_{nm}=C_n(\hat{z})C_m{}^\dagger(\hat{z})$ [Eq. (6)] and only $4S$ real numbers are required to determine the state of the ensemble. In the general case, however, $4S(S+1)$ real numbers are required to determine the state.[10]

By means of Stern-Gerlach magnets and Feynman filters, the ρ_{nm} are determined by the methods discussed in the last section; ρ_{nn} is the probability of finding S_z having the value n. If in the Feynman filter discussed in the last section only the gates n and m are left open, then the density matrix for those systems which pass through the filter is[9]

$$\rho'=\sigma\rho\sigma/\mathrm{Tr}(\sigma\rho\sigma), \tag{10}$$

where

$$\sigma=|\hat{z},n\rangle\langle\hat{z},n|+|\hat{z},m\rangle\langle\hat{z},m|. \tag{11}$$

[5] R. P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics* (Addison-Wesley Publishing Company, Reading, Mass., 1965), Vol. III, Chap. 5.

[6] For these measurements, the beam would have to be bent from its original x direction, say, to the z direction; we assume this done in such a way that the spin state is unaltered.

[7] See, for example, M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957), Chap. IV.

[8] V. Fano, Rev. Mod. Phys. **29**, 74 (1957).

[9] J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (Princeton University Press, Princeton, N. J., 1955), Chap. 6. See also Fano, Ref. 8.

[10] A particle of spin S may have nonvanishing multipole moments up to order 2^{2S}. The average values of the $4S(S+1)$ multipole components determine the spin state (see Fano, Ref. 8).

Analyzing the mixture (10) by a Stern-Gerlach apparatus in the x-y plane [see discussion preceding Eq. (8)], we obtain for the probability of finding $\mathbf{S}\cdot\hat{r}$ to have the value p:

$$\mathrm{Tr}(|\hat{r},p\rangle\langle\hat{r},p|\rho')=N\{(d_{pm}{}^{S})^2\rho_{mm}+(d_{pn}{}^{S})^2\rho_{nn}+2d_{pm}{}^{S}d_{pn}{}^{S}|\rho_{mn}|\cos[(m-n)\phi+\phi_{mn}]\}, \quad (12)$$

where $N^{-1}=\rho_{mm}+\rho_{nn}$ and $\rho_{mn}=|\rho_{mn}|\exp i\theta_{mn}$. Measurement of the diagonal elements (ρ_{mm} and ρ_{nn}) together with the measurements represented by (12) at two different ϕ's determine $|\rho_{mn}|$ and θ_{mn}.

Space. The method analogous to that above when applied to the density matrix in space is of course extremely impractical, but it does furnish a method which could in principle determine the density matrix. We sketch the method in Appendix B.

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APPENDIX A: MEASUREMENT OF CURRENT

There are several ways to measure the probability current. The probability current of an electron in an atom, say, is proportional to the electrical current, and the electrical current may be detected by means of its effect in scattering charged particles or neutrons, or in photon emission or absorption. Rather than considering such realistic methods of current determination, it is interesting to consider a simple *gedanken* experiment which in principle can be used to determine $\mathbf{j}(\mathbf{r})$ by a measurement of $\langle\mathbf{v}(\mathbf{r})\rangle$.

To determine $\mathbf{j}(\mathbf{r}_0)$, we first determine that the particle is in a small volume ω containing $\mathbf{r}_0$. We then measure its subsequent velocity. Upon repeating the experiment on many members of the ensemble, we obtain $\langle\mathbf{v}(\mathbf{r}_0)\rangle$. The current is $\rho(\mathbf{r}_0)\langle\mathbf{v}(\mathbf{r}_0)\rangle$.

When we determine that the particle is in ω, then, according to Heisenberg, we will give the particle an undeterminable impulse on the order of $[\langle(\Delta\mathbf{p})^2\rangle]^{1/2}=\hbar\omega^{-1/3}$. There is no principle of quantum mechanics, however, which prevents us from carrying out the position measurement in such a way that $\langle\Delta\mathbf{p}\rangle=0$. If such measurements are made for successively smaller ω's, then the subsequent velocity distribution curve will become increasingly broader, but the mean velocity will approach a limit.

Mathematically, if

$$\psi(\mathbf{r})=R(\mathbf{r})\exp[iS(\mathbf{r})\hbar^{-1}] \quad (A1)$$

is the wave function before the position measurement, then the wave function after the measurement will be

$$\psi'=Nf_\omega(\mathbf{r})R(\mathbf{r})\exp(iS\hbar^{-1}), \quad (A2)$$

where N is a normalization factor, and $f_\omega(\mathbf{r})$ is a *real* function which vanishes except for $\mathbf{r}$ in ω. It then follows that

$$\langle\psi'|\mathbf{p}|\psi'\rangle=\nabla S(\mathbf{r}_0) \quad (A3)$$

if ω is sufficiently small that $S=S(\mathbf{r}_0)+(\mathbf{r}-\mathbf{r}_0)\cdot\nabla S(r_0)$ in ω. But $\langle\psi'|\mathbf{p}|\psi'\rangle=m\langle\mathbf{v}(\mathbf{r}_0)\rangle$; thus the probability current $\mathbf{j}(\mathbf{r}_0)=\rho(\mathbf{r}_0)m^{-1}\nabla S(r_0)=\rho(\mathbf{r}_0)\langle\mathbf{v}(\mathbf{r}_0)\rangle$.

APPENDIX B: METHOD FOR DETERMINATION OF THE DENSITY MATRIX

The method utilized in Secs. II and III for determining the density matrix by first filtering out two components of the Hilbert space, then making a measurement wherein the two states interfere, is one which may generally be employed.

In order to determine the density matrix $\rho(\mathbf{x},\mathbf{x}')$ of a system consisting of a single spinless particle we could first determine that the particle is either at $\mathbf{x}_1$ or $\mathbf{x}_2$ without determining which. (This could be done by illuminating all space except for small regions containing $\mathbf{x}_1$ and $\mathbf{x}_2$ and eliminating all cases in which the particle is discovered in the illuminated region.) Subsequent detection of the particle on a closed surface surrounding $\mathbf{x}_1$ and $\mathbf{x}_2$. with measurement of both position and time, serves in principle to determine $\rho(\mathbf{x}_1,\mathbf{x}_2)$. If before the position measurement

$$\rho=\int d\mathbf{x}d\mathbf{x}'\rho(\mathbf{x},\mathbf{x}')|\mathbf{x}\rangle\langle\mathbf{x}'|, \quad (B1)$$

where $|\mathbf{x}\rangle$ indicates a position eigenket, then after the measurement the density matrix would be

$$\rho'=C\{\rho(\mathbf{x}_1,\mathbf{x}_1)|\mathbf{x}_,\rangle\langle\mathbf{x}_,|+\rho(\mathbf{x}_2,\mathbf{x}_2)|\mathbf{x}_2\rangle\langle\mathbf{x}_2|+\rho(\mathbf{x}_1,\mathbf{x}_2)|\mathbf{x}_1\rangle\langle\mathbf{x}_2|+\rho(\mathbf{x}_2,\mathbf{x}_1)|\mathbf{x}_2\rangle\langle\mathbf{x}_1|\}. \quad (B2)$$

In (B2), C is a normalization constant which we shall neglect hereafter since we are only concerned with the relative density distribution. Now the probability density for finding the particle at $\mathbf{x}$ after a time t if (B2) holds at $t=0$ is

$$P(\mathbf{x},t)=\rho(\mathbf{x}_1,\mathbf{x}_2)|G_t(\mathbf{x},\mathbf{x}_1)|^2+\rho(\mathbf{x}_2,\mathbf{x}_2)|G_t(\mathbf{x},\mathbf{x}_2)|^2+2\mathrm{Re}\rho(\mathbf{x}_1,\mathbf{x}_2)G_t(\mathbf{x},\mathbf{x}_1)\bar{G}_t(\mathbf{x},\mathbf{x}_2), \quad (B3)$$

where $G_t(\mathbf{x},\mathbf{y})=\langle\mathbf{x}|e^{-iHt}|\mathbf{y}\rangle$ is the Green's function for propagation from $\mathbf{y}$ to $\mathbf{x}$ in the time t. It is clear that measurements of $P(\mathbf{x},t)$, $\rho(\mathbf{x},\mathbf{x})$, together with the knowledge of the Green's function, would in principle furnish a means of obtaining the amplitude and phase of $\rho(\mathbf{x}_1,\mathbf{x}_2)$.