Measuring the quantum mechanical wave function

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In the past few years experimenters have learned how to determine the complete quantum state of an ensemble of particles or fields which have been prepared according to some unknown procedure. Through these experiments they have answered a question posed by W. Pauli in the 1930s. The methods used involve measuring statistical distributions of a well chosen set of physical observables and using a tomographic inversion algorithm to reconstruct the Wigner function and its corresponding wave function or density matrix. Recontructions have been successfully carried out in atomic, molecular, and optical physics. The development of these procedures helps to firm up the interpretation of the Schrödinger wave function.

1. Introduction — the Pauli question

Since the early days of quantum mechanics (QM) there has been puzzlement over the physical meaning of Schrödinger's wave function $\psi(r)$. Is it analogous to other fields in nature, such as the gravitational or electric fields? Probably not — these are physical fields, which represent concrete forces and thus can be directly measured by using a suitable instrument designed to respond to these forces. Nevertheless, many scientists (and non-scientists) have elevated the ψ-field in their thinking to represent some reflection of reality that can be associated with the particle that it is meant to represent. Some would even replace the particle itself by its mathematical ψ representation. But wait. Max Born told us in the 1920s that the square of the ψ-field, $\left|\psi(r)\right|^2$ actually represents only the probability for an experimenter to observe, or find, the particle near a location r if she uses a suitable instrument to detect its presence. Any QM textbook will tell you that, and it is perfectly true as far as anyone presently knows.

But what of $\psi(r)$ itself? Why is it a complex number, composed of 'real' and 'imaginary' parts, $\psi_R(r) + i\psi_I(r)$? The surprising truth, I believe, is that at this point we do not know *why* ψ has two parts [1]. The good news is that we do know almost everything about how to calculate ψ for a given physical set up. We know how to use the calculated ψ to predict the outcomes of the most excruciatingly detailed measurements — for example the gyromagnetic ratio of the electron is known experimentally and theoretically to twelve significant digits [2].

We know all of this about $\psi(r)$, but do we know how to 'measure' it? Since $\psi(r)$ is not a physical field, we *cannot* construct a ψ-meter, much like a volt – ohm meter, which would register a definite value of ψ on interacting with a particular quantum system (perhaps a particle) in question. See figure 1. If you adopt Born's assertion, you realize that in order to measure (that is, determine by experiment) the squared function $\left|\psi(x)\right|^2$ it is sufficient to do the following. Prepare in an identical fashion a very large number (M) of identical systems and, one-after-the-other, measure their
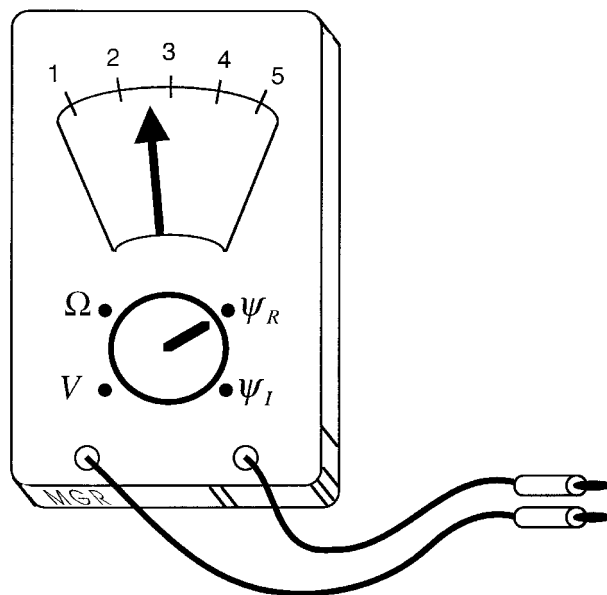

Figure 1. A hypothetical meter which, by choosing the proper setting, would measure volts, ohms, or the real or imaginary parts of the ψ-field.

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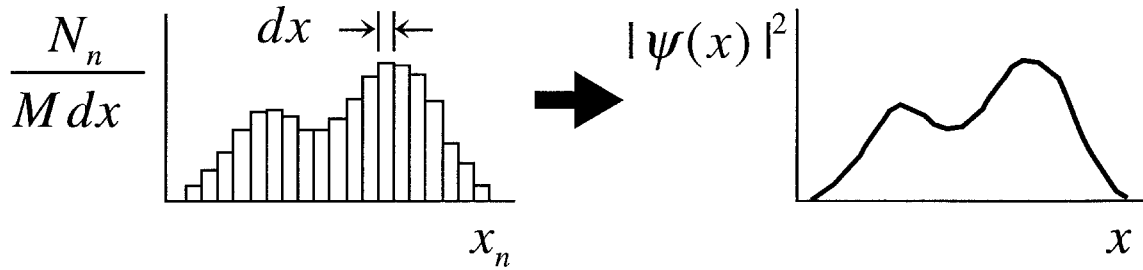
Figure 2. A histogram of event numbers becomes an experimental estimate of the square of the wave function ψ as the size of each bin becomes small and the number of measurements becomes large.

positions x_n, for $n = 1, 2, \ldots, M$. (I am using one dimension only, for simplicity). Then build a histogram, as in figure 2, of the number N_n of times that x_n falls within a range x to $x + dx$, and assert that the probability density, or $|\psi(x)|^2$, is proportional to N_n/M that is,

$$|\psi(x_n)|^2 \, dx \cong N_n/M. \tag{1}$$

Other than the use of the notation $|\psi(x)|^2$ for probability density, this procedure is the same as that used in purely classical statistics. For example, if you sum over N_n/M, or integrate over $|\psi(x)|^2$, you must get unity. In light of this, it is probably more clear to say that you have 'inferred' or 'determined' $|\psi(x)|^2$ rather than 'measured' it, since a single observation of a particle tells virtually nothing about the whole form of $|\psi(x)|^2$.

We arrive at a conclusion and a question. The ψ-function is a statistical property of (or represents probablity information about) a very large collection of similarly prepared particles rather than a single particle. The very concept of a wave function of a single particle can be called into question, as I will discuss below. The question still is — can I infer the whole complex fuction $\psi(x)$ from some series of measurements on a large collection of identically prepared particles? This is a generalized version of the 'Pauli Question' [3].

In the following I will explain how this generalized Pauli Question has recently been answered in the affirmative. I will discuss recent experiments which allowed the inference of ψ corresponding to the quantum states of a vibrating molecule, a trapped atomic ion oscillating in a confining potential, a light field, and an atomic beam.

2. The structure of quantum mechanics — the key to 'measuring' ψ

The key to the Pauli Question turns out also to contain one of the biggest mysteries of QM — the wave function $\psi(x)$, describing the particle's position information, is uniquely related to the wave function, $\widetilde{\psi}(P)$, describing its momentum (P) information. There is no counterpart to this statement in classical (Newtonian) physics. It means that the relation between momentum and position probability densities is not arbitrary, as it would be if the world were classical. It is telling us that momentum and position are not completely independent quantitites nor even wholly separate concepts. In some sense they could be thought of as two different, complementary properties, or aspects, of a single underlying entity, or element of reality. This thought is the key to solving our problem because it leads us to the idea that we must reconstruct an underlying structure of information about the particles which itself cannot be directly observed. This information structure, as I am calling it, is the quantum wave function.

With this background I will now give a tentative, but completely standard, definition of 'ψ-function', or more generally 'quantum state'. Paraphrasing Ballentine [4,5], I assert.

(1) A quantum state of a physical system (e.g. particle) is that which specifies the probability distributions for measurements of any and all physical, observable quantities pertaining to that system.

(2) The state may be associated with an abstract (and infinite) collection of systems which are all created or prepared in an identical way.

(3) Mathematically the state may be fully represented by the Schrödinger ψ-function (in the case of identical system preparation).

(4) In the case of non-identical preparation the description may be generalized by using the so-called density matrix, or state matrix.

Item (1) generalizes the fact, pointed out earlier, that the momentum and position distributions can be found from the same wave function $\psi(x)$. That is, the momentum wave function is

$$\widetilde{\psi}(P) = \frac{1}{(2\pi\hbar)^{1/2}} \int \psi(x) \exp -(ixP/\hbar) \, dx, \tag{2}$$

namely, a Fourier transform of ψ. (Unless stated, all

integrals are from $-\infty$ to $+\infty$. The generalization of equation (2) to an arbitrary variable R is

$$\widetilde{\psi}_R(R) = \int \psi(x)\, U(x, R) \, \mathrm{d}x, \qquad (3)$$

where $U(x, R)$ is some transformation function. Then the probability density for obtaining values R upon measurements is $\left| \widetilde{\psi}_R(R) \right|^2$.

It is not understood deeply *why* the wave functions transform in this way. This question is likely related to the question why the wave function is complex. Again the complementarity idea comes in. Any two variables whose wave function representations transform as in equation (2) are said, first by Niels Bohr, to be complementary [6].

If the state if identified with the set of probability densities for *all* possible observable variables, as in Item (1), then it might be thought that in order to determine a state, you would need to measure the distributions of *all* of the variables and then try to invert the data to find the state. It turns out, though, to our good fortune, that one needs only to measure the distributions of a subset of all possible variables. I call such a subset of variables Tomographically Complete.

I want to clarify that the Pauli Question does not deal with determining the familiar energy eigenstates of a quantum system, a task familiar from textbooks and which makes up the core of spectroscopy. Rather Pauli asked how to determine the particular linear combination of eigenstates that a system has been prepared in.

3. Reconstructive tomography — classical

Tomography generally means the reconstruction of an unknown two-dimensional (2-D) function $D(x, y)$ from knowledge of a large set of one-dimensional functions, called projections, which are related to the 2-D function by adding up, or integrating, its values along a set of paths, often straight lines [8]. You should know this concept from medical imaging — a medical technician passes beams of X-rays through a 2-D slice of your body, which absorbs the
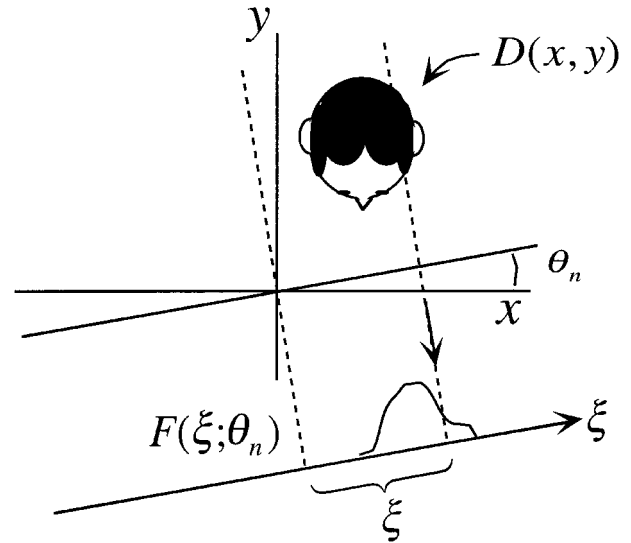
'In quantum physics . . . evidence about atomic objects obtained by different experimental arrangements exhibits a novel kind of complementarity relationship. Indeed it must be recognized that such evidence, which appears contradictory when combination into a single picture is attempted, exhausts all conceivable knowledge about the object. . . . Moreover, a completeness of description like that aimed at in classical physics is provided by the possibility of taking every conceivable experimental arrangement into account.' [7]

Niels Bohr

Figure 3. In computer-aided tomography (CAT) a beam of X-rays passes through a head, integrating the head's density function $D(x, y)$ along straight lines. If this is carried out for many different angles θ_n the density function can be reconstructed by computer processing of the projection data.

X-rays, adding up the density of the bits along different straight paths, to produce a 1-D function $F(0, x)$. Your body is then rotated by various angles θ_n and the process is repeated to yield a set of functions $F(\theta_n, \xi)$ where ξ is the distance from the origin to the line of integration. This is illustrated in figure 3. Finally the set of functions is used to reconstruct the original 2-D density function $D(x, y)$, thereby producing an image of the interior 2-D slice of your body. For discovering and applying this inversion method to medical imaging in the 1960s, Cormack and Hounsfield shared the Nobel Prize in Medicine. The underlying mathematics had been previously discovered by Johann Radon in 1917. The so-called Radon transform (RT) and its inverse are operations that can be performed by computer software, and can be expressed as

$$F(\theta_n, \xi) = RT\left\{ D(x, y) \right\}, \qquad (4)$$

$$D(x, y) = RT^{-1}\left\{ F(\theta_n, \xi) \right\}, \qquad (5)$$

How can we apply this type of reasoning to momentum and position measurements? Think of a collection of particles having classical behaviour — say muffins coming rapidly down a flat-surfaced chute in an automated muffin factory†, as in figure 4.

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†This may remind some readers of the Utility Muffin Research Kitchen described by F. Zappa. ['Muffin Man', by F. Zappa, in *Bongo Fury* (Warner Bros., Los Angeles, (1975)]
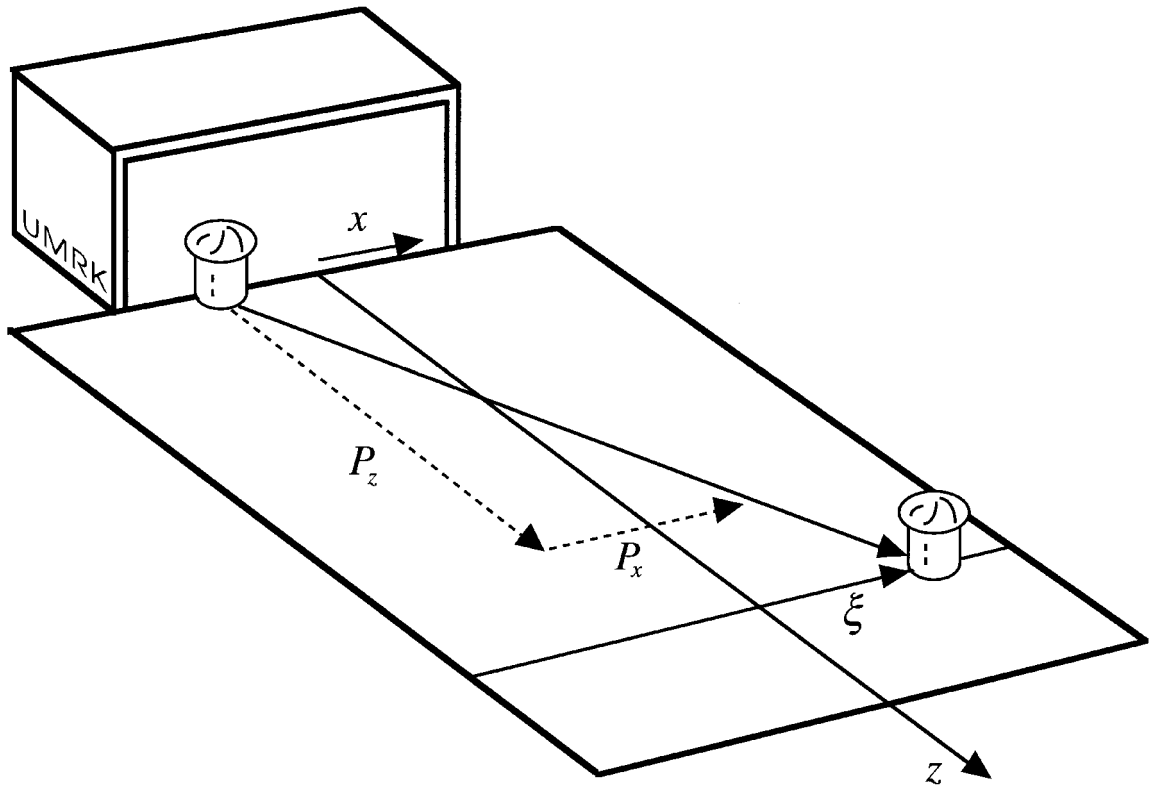
Figure 4. An ensemble of classical particles (illustrated by muffins) exit in random directions from an oven at $z = 0$. Our goal is to determine the joint-probability density Pr (x, P_x) for muffin position x and momentum P_x without measuring both position and momentum for any single muffin.

Assuming the laws of statistics are in effect, there is some joint-probability density Pr (x, P_x) for muffin position x and momentum P_x in the x-direction. How can you find out this 2-D density function by making measurements of only 1-D density functions? The tomographic method gives the answer — simply measure the position distribution at many different distances, L_n, from the oven source. Call each distribution $F(\xi; L_n)$, with ξ being the position variable. If the speed in the z-direction is much larger than that in the x-direction, and is equal for all muffins, the observed position ξ will be given in terms of the unknown x and P_x values by $\xi = x + (P_x/m)t$, where m is the muffin mass and $t = L_n m/P$ is the time taken to move to the $z = L_n$ line. The fraction (probability) Pr $(\xi; L_n)$ of muffins arriving at ξ will be proportional to the sum number of all muffins having the correct *combination* of initial x and P_x so that they each arrive at ξ. That is, for each L_n,

$$\text{Pr } (\xi; L_n) = \int\!\!\int_{C(\xi)} \text{Pr } (x, P_x) \, \mathrm{d}x \, \mathrm{d}P_x, \qquad (6)$$

where the $C(\xi)$ means an integral through the (x, P_x) plane along the line made up of all points satisfying $x + (P_x/m)t = \xi$ (ξ fixed), as shown in figure 5. Equation (6) is a

case of the Radon projection transform and so we know that it can be inverted as in equation (5) if we can measure a sufficient number of the Pr $(\xi; L_n)$ functions at different L values. By this method the initial density function Pr (x, P_x) is obtained!
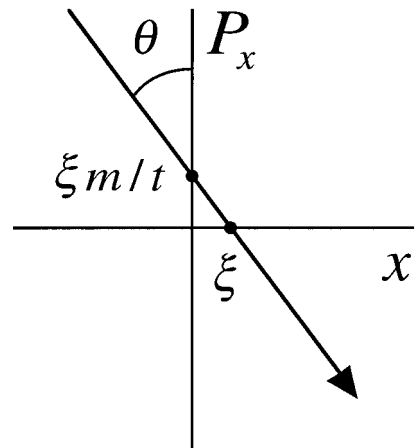

Figure 5. The line of integration defining the probability Pr $(\xi; L_n)$ of a particle arriving at ξ, according to equation (6).

4. Reconstructive tomography — quantum

This ability to extract 2-D, or joint, probabilities pertaining to a pair of random variables from measurements only of individual random variables is quite nice and can be applied to data similarly measured for a stream of quantum particles. These could be atoms emitted from a 'hot-oven' source. You may have guessed already the reason for this strange-appearing scheme. We all know that Heisenberg's indeterminacy principle (often mistranslated as 'uncertainty' principle) states that it is not possible, even as a matter of principle, to measure simultaneously, or jointly, the momentum *and* position of an individual particle with arbitrarily high precision. (This is related to the idea of complementarity, discussed earlier, and a similar statement holds for any pair of complementary variables, those obeying equation (2)). Fortunately the proposed scheme requires us only to measure one variable — position — and this can be done with very high precision indeed [9]. So nothing can stop me from measuring the distributions Pr $(\xi; L_n)$ for a set of truly quantum particles. And no one can prevent me from entering this measured data into my computer which contains the software to invert the Radon projection integral, to yield a 2-D function which I have previously called the joint probability, or Pr (x, P_x). But now I must not use this terminology since QM tells me that there is actually *no such thing* as a joint probability for complementary variables. So I will call it the computer-reconstructed function $W(x, P_x)$ instead of Pr (x, P_x).

What is the physical meaning of this reconstructed function $W(x, P_x)$? A near-miracle occurs at this point because it turns out that from this 2-D function I can numerically construct not only the square of the wave function, but the actual complex wave function of Schrödinger! To put this into context, it helps to back up a little and discuss an important contribution made by a great physicist, Eugene Wigner.

5. The Wigner quasi-probability distribution

Besides making important theoretical advances in a wide range of physics, Wigner is known for his introduction of an interesting way to see the correspondence, or rather lack of correspondence, between classical and quantum theory. In struggling with certain problems in statistical thermodynamics he was inspired to try to write the quantum version of the equations in a form as similar as possible to those in the classical theory. To do this he wanted to find a way to use Schrödinger's wave function $\psi(x)$ to write an expression which has the look and feel of a joint probability for momentum and position. Realizing that no true function of this type could exist, he (or perhaps others later) began to call his new function a quasi-probability distribution.

Wigner defined the following function [10],

$$W(x, P_x) = \frac{1}{2\pi\hbar} \int \psi(x + x'/2) \psi^*(x - x'/2) \exp(-ix'P_x/\hbar) \, dx'. \quad (7)$$

Notice the similarity between this transformation and equation (2). Both are Fourier transforms from position to momentum. But because the integral in equation (7) is over x', the x variable still appears as a variable in $W(x, P_x)$.

Here is the key point. It turns out that the quantum tomography procedure I described above reconstructs exactly the function $W(x, P_x)$ in equation (7). To see the tomographic connection first try integrating equation (7) over P_x. Recall the fact that integrating $\exp(-ix'P_x/\hbar)$ over P_x yields a Dirac delta function of x', that is a function which is zero everywhere other than at $x' = 0$ [11]. This means that the following x' integration just picks out the value of the integrand $\psi(x + x'/2) \psi^*(x - x'/2)$ at the value $x' = 0$, giving

$$\int W(x, P_x) \, dP_x = |\psi(x)|^2. \quad (8)$$

This says that the correct quantum probability for position x is obtained by integrating the 2-D function $W(x, P_x)$ in the x, P_x plane along the line on which x is held constant. That is a special case of the projection integral illustrated in figure 5, in the case that the line is vertical (parallel to the P_x) axis. So equation (8) is an example of the Radon projection integral.

Another projection example can be found by integrating $W(x, P_x)$ over the x variable. A similar (but trickier) calculation leads to

$$\int W(x, P_x) \, dx = |\tilde{\psi}(P_x)|^2, \quad (9)$$

where $\tilde{\psi}(P_x)$ is the momentum wave function given in equation (2). So equation (9) gives the measurable distribution for momentum, and is related to $W(x, P_x)$ by a horizontal-line integral in figure 5. It turns out that the distributions of all measurable variables $\xi = x + (P_x/m)t$ are equal to projection integrals along precisely the same lines as are proper in the classical case. That is, if a ξ-wave function $\tilde{\psi}_\xi(\xi)$ is calculated using the correct transformation equation (3), then the probability distribution for the ξ variable is expressible as

$$\int_{C(\xi)} \int W(x, P_x) \, dx \, dP_x = |\tilde{\psi}_\xi(\xi)|^2. \quad (10)$$

This naturally means that we can reconstruct the Wigner function $W(x, P_x)$ by applying the inverse-Radon software to the validly collected set of distributions Pr $(\zeta; L_n)$. This is quantum tomography. This was first proved by the wife-and-husband team of mathematical physisicts J. Bertrand and P. Bertrand [12].

One proof that $W(x,P_x)$ cannot be a classical joint probability is the fact that for certain quantum states it can take on negative values for some values of x and P_x. In contrast, true probabilities must be positive.

How do we find the wave function once we know the Wigner function? Because the equation is a Fourier transform it has a unique inverse; this yields the product $\psi(x+x'/2)\ \psi^*(x-x'/2)$, which can be thought of as a complex function in the x,x' plane. By evaluating this function along the line $x=x'/2$ we obtain $\psi(2x)\psi^*(0)$. We know that any wave function may be multiplied by an arbitrary phase factor $\exp(i\phi)$ without changing the physical state — this is the meaning of the factor $\psi^*(0)$. Thus, by dividing $\psi(2x)\psi^*(0)$ by $[\psi(0)\psi^*(0)]^{1/2}$ we obtain $\psi(x)$ to within an arbitrary phase.

Why, or how, does this work? How can measuring real functions of single variables yield a complex function? Again it is due to the remarkable structure of QM itself. The distributions of all of the measurable variables ξ can be computed from a single complex, 1-D function $\psi(x)$, or alternatively from the single real, 2-D function $W(x,P_x)$. These functions are uniquely related to one another.

6.   Quantum to classical

If the experiment described above is carried out with muffins, instead of single atoms, do we obtain a ψ-function for the muffins, which after all are classical bodies? No! A collection of real muffins could most likely *never* be prepared in a pure quantum state the way atoms can. This is because muffins (like cats or dogs) are far too large and complicated for mere mortals to be able to prepare them perfectly, *and identically*, every time. Many outside influences interfere — a flea sneezes, a photon goes bump, a proton decays, all disturbing the preparation process. It is now understood better than it was in the 1920s why small influences are actually far more severe for large bodies than for tiny ones. It has been shown that a wide class of influences that can be associated with random events will lead to the destruction of the coherence between different parts of a wave function [13]. The farther apart (in phase space) that these pieces of the wave function are, the faster the coherence is destroyed, and by tinier amounts of outside influences. If there were truly *no* outside influences (the muffin or cat is in a shielded box at absolute-zero temperature) then in principle a macroscopic system prepared in a particular ψ state would remain in that state. But in reality any random outside influence, even just the tidal-induced distortion of the moon and its consequent gravitational interaction with our muffin of interest (you cannot shield gravity) will cause the 'decoherence' of its wave function [14].

If we prepare a collection of large, macroscopic particles to the best of our ability they will not be described by a single, pure quantum state — therefore a quantum-tomography reconstruction experiment will not produce such a pure state. Rather, a statistical mixture of many possible states will be found. Mathematically this is represented by a so-called density matrix, which can describe a quantum system or a system having almost perfectly classical statistical properties [15]. It also turns out that in this case the Wigner function may well be thought of as being truly a classical joint probability distribution; it is positive for all values of x and P_x. One might even argue that all classical probabilities are actually Wigner functions in the classical limit.

If we prepare a collection of microscopic particles (not muffins) which are well isolated from their environment then we can approach the ideal limit in which the ensemble is described by a pure quantum state. Unavoidable, slight deviations from this limit, caused by small imperfections in our preparation procedure, will not prevent us from approximating the ideal case, and therefore in this limit we can say we have reconstructed a pure state for all practical purposes.

7.   Case studies of quantum tomography

Only since 1993 have measurements been performed for the purpose of reconstructing quantum states for the behaviour of a continuous degree of freedom, like position. In this section I will describe all of the examples of such measurements that have been carried out to date. They are: free particles, molecular vibration, trapped-ion motion, and a light field†.

7.1. *Vibrating molecule — the harmonic oscillator*

Two atoms bound chemically form a simple molecule, as in figure 6. Denote the distance between the atoms by q and the momentum associated with its change by p. Initially the electrons and nuclei are in their lowest energy eigenstate. A short laser pulse can be used to excite the electron cloud to a higher energy eigenstate. As a result the nuclei suddenly feel new forces and their separation distance q begins to oscillate. The restoring force can be approximated by $-kq$ (k is the spring constant), corresponding to motion in a harmonic potential $\frac{1}{2}kq^2$. We can describe the vibrations of the initially excited state (a wave packet) by using the well known quantum theory of the harmonic oscillator. The

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†A few years earlier quantum states for angular-momentum of an electron in an atom were obtained experimentally [17]. Because the angular momentum of these states involved only a few discrete values, a smaller number of measured distributions is required than in the continuous case, and the tomographic analogy does not hold in a simple way. Nevertheless, the role of reconstruction is the same.
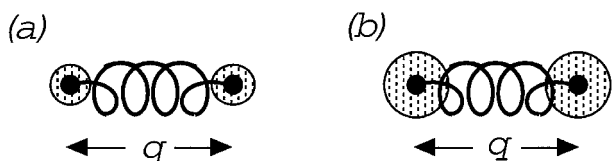
Figure 6. (*a*) Two atoms with internuclear distance *q* and electrons in their lowest energy state form a molecule. (*b*) An ultrashort laser pulse excites the electrons to a higher-energy state, which induces the nuclei to begin vibrating.

time evolution of the Wigner function is governed by the time-dependent Schrödinger equation. Only the harmonic oscillator and the free particle have the remarkable property that their quantum Wigner functions $W(q,p)$ evolve in time exactly as do their corresponding clasical joint probabilities Pr (q,p) for position and momentum [16]. This happy accident means that we can again appeal to a classical picture to understand the dynamics.

A classical harmonic oscillator with initial position q_0 and initial momentum p_0 evolves in time harmonically:

$$q(t) = q_o \cos \omega t + (p_o/\omega m) \sin \omega t,$$
$$p(t)/\omega m = -q_o \sin \omega t + (p_o/\omega m) \cos \omega t, \quad (11)$$

where $\omega = (k/m)^{1/2}$ is the natural oscillation frequency. If this is plotted as a curve in a q, $p/\omega m$ plane, it traces out a circle. A whole distribution of initial $(q_0, p_0/\omega m)$ points will therefore simply rotate with time in the q, $p/\omega m$ plane without changing its shape. This is shown in figure 7. As seen in the figure the probability distribution Pr $(q;t)$ for q oscillates back and forth, changing shape periodically. Because Pr $(q;t)$ is given by the Radon projection integral along vertical lines (dashed in the figure), we again have a basis for tomography, quantum or classical.

This type of state reconstruction has been performed with sodium molecules by Dunn *et al* [18]. After exciting the molecular vibration with a laser-pulse, these researchers measured the spectrum of light emitted by the molecules as they oscillated. By observing the time evolution of this spectrum they could determine, with some finite precision, the probability distribution Pr $(q;t)$. From this they reconstructed an image of the Wigner distribution shown in figure 8, representing the state of the molecular vibration just following the excitation pulse. Actually, because of the finite resolution of the Pr $(q;t)$ measurements, the function shown in the figure is really a blurred image of $W(q, p)$. For this reason the researchers were not able to proceed to extracting the complex wave function. Nevertheless, the measurements still provide the most detailed characterization of any molecular vibration yet achieved. This type of information should be helpful in current efforts to create specific wave-packet states of molecules for the purpose of controlling chemical reactions.
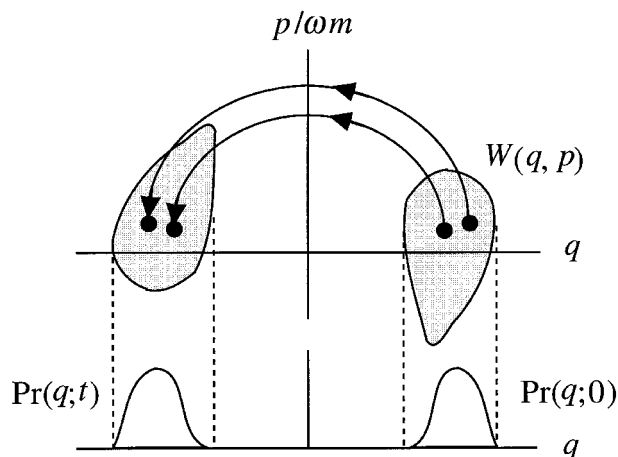

Figure 7. The motion of the molecular oscillator is shown in a phase space made up of the interatom separation *q* and the interatom momentum *p*. The Wigner function, which represents the quantum state, rotates in this space, and the projected Wigner function, equal to the probability distribution Pr (*q*;*t*) for *q*, oscillates.
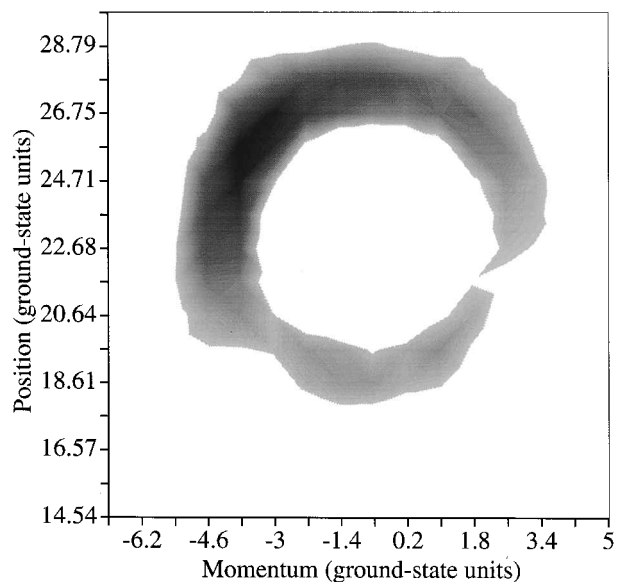

Figure 8. The result of an experimental reconstruction of a Wigner function (with some blurring) representing the quantum state of a molecular oscillator. (From [18].)

7.2. *Light — a harmonic EM oscillator*

The properties of light provided some of the earliest hints about the quantum nature of the world. Einstein's interpretation of the Planck blackbody spectral formula really kicked things off. What is light, though? We know from Paul Dirac's theoretical work that light is the quantized excitations of the electromagnetic (EM) field. A

linearly polarized, plane travelling wave can be represented at a fixed point in space by its oscillating electric-field amplitude,

$$E(t) = E_0[q \cos(\omega t + \theta) + p \sin(\omega t + \theta)]. \quad (12)$$

Here E_0 is a known scaling field value that depends on the volume of the enclosure in which the light travels and Planck's constant $\hbar$. Here the variables called q and p have nothing to do with position or momentum; they are simply unitless numbers giving the strength of the electric field. The notation reminds us that q and p are complementary in the sense of equation (2). Also an optical phase shift θ is included in equation (12). Let us denote by q_0 and p_0 the values in the special case that $\theta = 0$. If the value of the phase shift is not zero, then q, p may be related to q_0 and p_0 by

$$q = q_0 \cos \theta + p_0 \sin \theta,$$

$$p = -q_0 \sin \theta + p_0 \cos \theta. \quad (13)$$

This has a form similar to equation (11) and it also describes a simple rotation in the q, p plane. Again we can carry out quantum tomography; we need only to measure the probabilities Pr $(q;\theta)$ for observing a (unitless) electric-field strength q, for many values of phase shift θ between 0 and π.

Measurements of the field strength in a light beam can be performed by using interferometry. The unknown field of interest (the signal field) $E(t)$ is made to interfere with a known, much stronger, reference field $E_R(t)$, with

$$E_R(t) = E_{R0} \cos(\omega t + \theta). \quad (14)$$

The time-integrated intensity of the light after interference is given by

$$\frac{1}{T}\int_t^{t+T} [E_R(t) + E(t)]^2 \, dt = \frac{1}{2}E_0^2 +$$

$$\frac{1}{2}E_{R0}^2 (q^2 + p^2) + E_{R0}E_0 q. \quad (15)$$

If E_{R0} is much larger than E_o and known, then from a measurement of this intensity we can obtain the value of q. Notice that the value of θ is defined by a phase shift which can be introduced into the reference field and can be controlled by the experimenter.

Again we follow the tomographic scheme — measure q many times for each value of θ to build up histograms and thereby determine the set of probabilities Pr $(q;\theta)$ [19]. Because the θ values correspond to different rotations in the q,p plane we can apply the standard reconstruction mathematics and obtain the Wigner function $W(q,p)$. If the light field is prepared in a pure-wave-function state, this wave function can be determined from the reconstructed Wigner function.
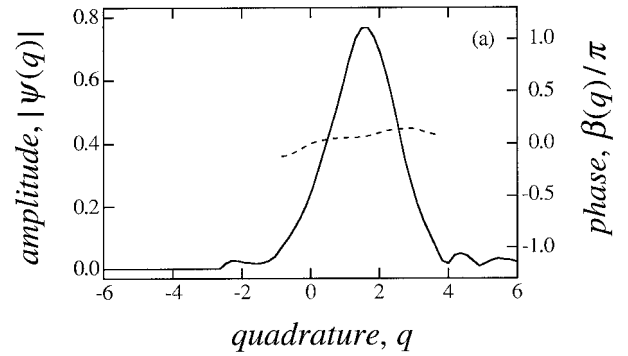

Figure 9. An experimentally reconstructed quantum wave function of a pulsed light field containing on average 1·2 photons, produced by strongly attenuating a laser field. The variable *q* is a unitless measure of electric-field strength, and $|\psi(q)|^2$ equals the probability for *q* to be found having a certain value. The wave function is expressed as $\psi(q) = |\psi(q)| \exp[i\beta(q)]$ where $|\psi(q)|$ is the amplitude (solid curve) and $\beta(q)$ is the phase structure (dashed curve). (From [20].)

The result of such a wave-function measurement carried out by researchers in my laboratory at the University of Oregon is shown in figure 9 [20]. A light beam from a stable laser was split on a partially reflecting mirror to provide the reference field travelling in one direction and the signal field in another. The signal was strongly attenuated using more reflective and/or absorbing surfaces in order to make a field weak enough to be subject to true quantum measurements. The two fields were again combined on a 50% reflecting mirror and the interference was measured, from which the value of q for each trial was obtained. After tomographic reconstruction of $W(q,p)$ the wave function shown in the figure was determined. It shows results expected for a coherent laser field — a constant, or linearly varying phase, and a smooth, Gaussian-like peak in the amplitude of the wave function, centred at a small non-zero value equal to the average value of q.

The mean value $\bar{n}$ of the photon number n in the light field is analogous to the average excitation quantum number of a harmonic oscillator and in both cases equals the expectation value of the energy divided by $\hbar\omega$ This is given by

$$\bar{n} = \int \psi^*(q)\frac{1}{2}\left(q^2 + \frac{d^2}{dq^2}\right)\psi(q) \, dq, \quad (16)$$

and has the value 1·2 in this example. Note that in the photon-number formula there are no factors of $\hbar$ or m as would appear for an oscillator with mass m.

Now a very interesting point can be made about the usefulness of this measurement scheme. We made only interferometric measurements on the signal field, so no precise information about the signal photon number could be obtained from a single measurement. Nevertheless we

obtained the wave function from which, according to Item (1) in the definition of quantum state, we can deduce the probability of *any* variable, even those which were never measured. We can use this idea to find the probability distribution Pr (*n*) for the photon number *n* in the field. Given the measured $\psi(q)$, this probability is simply given by

$$\Pr(n) = \left| \int \psi^*(q) u_n(q)\, dq \right|^2, \qquad (17)$$

where $u_n(q)$ is the familiar *n*th energy eigenfunction of the harmonic oscillator [21]. We plot Pr (*n*) in figure 10 for this example. Evidently this offers a new alternative to standard 'photon-counting' methods for measuring the probability for finding *n* photons in the field. In fact, for technical reasons relating to the efficiencies of different detector types, the tomographic method actually gives higher fidelity than does the standard one [22]. For example, it has been used recently to verify the presence of *photon pairs* in a light beam created by the 'splitting' of single green photons into pairs of infrared photons in a crystal [23].

7.3. *Ion in a trap*

A positive ion (an atom missing an electron) is a charged particle and can be trapped and held in one place indefinitely by using oscillating electric and magnetic fields [24]. The position of the ion oscillates harmonically in space around the centre of the trap where the energy is lowest. This ion motion obeys quantum mechanical laws and is thereby described by a quantum state. Recently experiments have been done to determine the state of an ion's motion [25]. A method related to, but not identical to, quantum tomography was used. At a certain time the centre of the trap was suddenly shifted to a new position and the probability that the ion ended up in the ground state of the shifted trap was measured. By shifting the trap centre to many different locations and making this type of measurement on an ensemble of ions, sufficient information could be obtained for a complete state reconstruction.

Clever laser techniques were used to prepare ions in the *n* = 1 vibrational energy eigenstate state of the trap potential. Then the above-described method was used to measure the state and verify the preparation process. The resulting reconstruction of the Wigner function for an ensemble of such ions is shown in figure 11. The remarkable feature of this Wigner function is the presence of negative values at certain points in *q, p* phase space. This means that $W(q, p)$ cannot be a joint probability and is proof that the
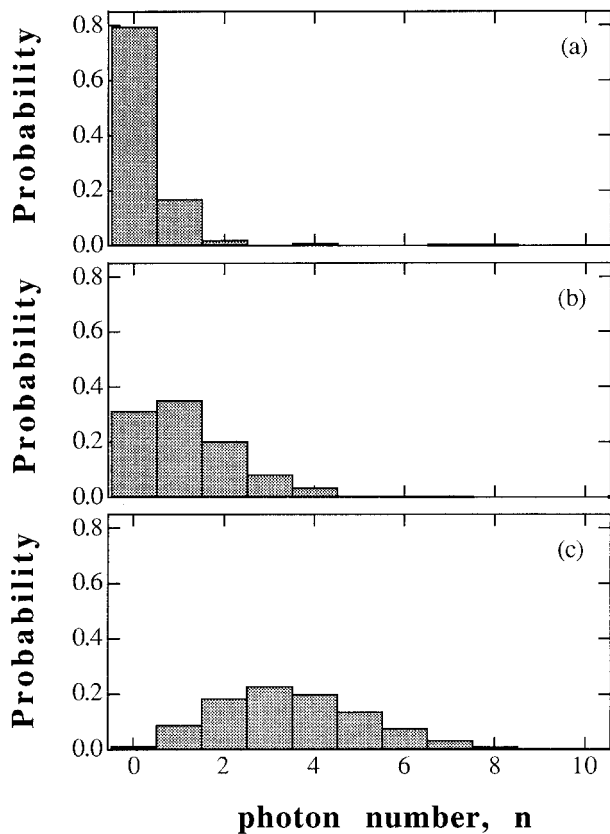

Figure 10. The photon-number probability distribution for a strongly attenuated laser field, as determined by inserting the measured wave function (for example, that shown in figure 9) into equation (17). Results are shown for coherent states containing on average (*a*) 0·2, (*b*) 1·2, and (*c*) 3·6 photons. (From [20].)
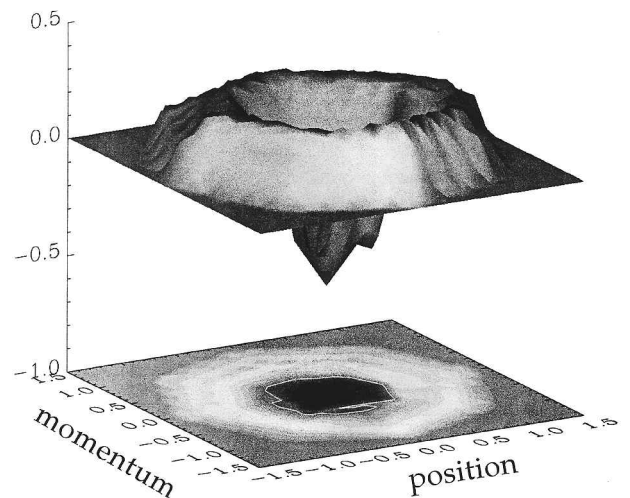

Figure 11. Experimentally reconstructed Wigner function $W(q, p)$ for motion of an ion in a trap. Momentum and position values have been divided by their corresponding root-mean-square values associated with zero-point motion. Negative-value regions indicate the absence of a classical description of the ion's motion. (From [25].)

motion of the ions is strongly quantum mechanical, with no classical correspondence.

7.4. *Free atoms and atom optics*

At the beginning of this paper we discussed the case of free particles, since it is conceptually the simplest. On the other hand the experiments in this case are not so simple and have not yet been successfully performed in a complete fashion. The source of the difficulty can be seen by going back to figures 4 and 5. While equation (6) correctly shows that the probability distribution for position ξ is given by a projection integral through the joint x, P_x probability, the actual range of possible projection angles is limited by the setup shown in figure 4. Because t is always positive in the relation $(P_x/m)t = -x + \xi$ defining the projection line, the angle between the P_x axis and the projection line can be only in the range 0 to $\pi/2$. In order to cary out the inverse Radon transform a range 0 to π is needed. This range can be accomplished by placing at some z-position a deflection device which acts like a lens for atoms [26]. This can be built using recently developed principles of atom optics: a focused laser beam shifts the potential energy and velocity of an atom in a spatially dependent way; so if the focus is properly shaped it can act as a lens for the de Broglie waves of the atomic motion [27]. You can convince yourself by an analysis of this geometry that the correct range of projection integrals can now be obtained [26,28].

Recently a beautiful experiment was performed in which a partial reconstruction of the Wigner function for free atoms was achieved [29]. The setup was similar to that shown in figure 4, except that a pair of closely spaced slits were placed in the beam at the location of the source. This produced the possibility of atom–wave interference and gave an interesting case worthy of reconstruction. A special 'camera' for atom imaging was used to record the atomic density pattern, averaged over many hours since at any one time only one or fewer atoms were present in the appartatus. The pattern was recorded at many different distances from the source, up to two metres. Data for only a limited range of evolution times (phase-space angles) were recorded (no lens was used). An incomplete inverse Radon transform was used to analyse the data; therefore the reconstructions cannot yield a true Wigner function. Still, the method does produce striking reconstructed 'Wigner-like' functions, one of which is shown in figure 12. The fine oscillations are a signature of quantum interference between the atom wave-function components emerging from the two slits. Within these oscillations are regions of negativity, indicating departure from a classical joint probability interpretation.

In spite of the technical difficulty, a complete reconstruction using atom lenses would be worth performing, as can be seen by thinking about the analogy between an atom beam and a light beam. We are fairly familiar with the ideas of spatial and temporal coherence of a classical light field.
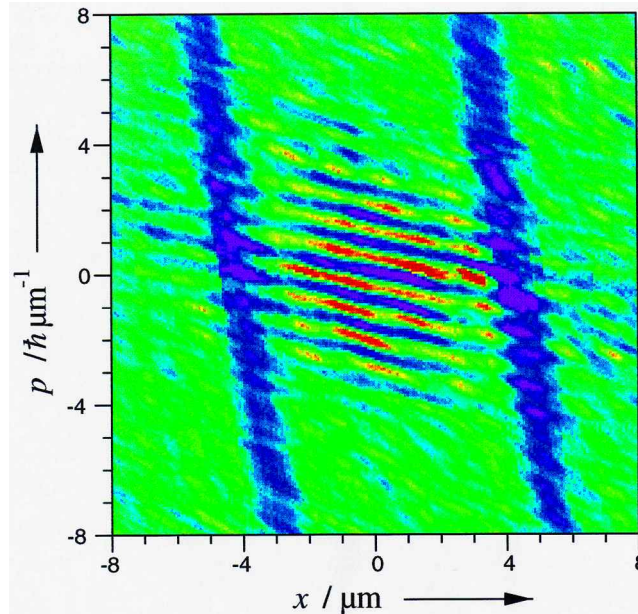

Figure 12. Experimental results of partial reconstruction of a Wigner-like function for free atoms after passing through a pair of closely spaced slits at the location of the source. Position x is given in units of microns (micrometres), and momentum p is given in units of Planck's constant divided by microns. Evidence of the two slits is seen as the two dark bands running nearly vertically (localized in x). Quantum interference effects are present as the rapidly oscillating structure near the centre, which contains both positive and negative parts. (From [29].)

Such coherence tells us about the relative timing, or phase, of the electric (E)-field oscillations at two separated space points x_1 and x_2, and about whether this relative phase changes with time. Mathematically this can be quantified by the product of the field $E(x_1)$ times the complex conjugate $E^*(x_2)$, averaged over all possible values of E and E^*; this is expressed as $\langle E(x_1)E^*(x_2)\rangle$, and is called a correlation function. If the field is written as $E(x) = A(x)\exp[i\beta(x)]$ then the correlation function is $\langle A(x_1)A(x_2)\,exp\,[i\{\beta(x_1)-\beta(x_2)\}]\rangle$ and depends on the phase difference $\beta(x_1)-\beta(x_2)$.

For an atom beam the analogue of the correlation function is given in terms of the set of possible wave functions which might correspond to the states of subsets of atoms. This analogue is $\langle\psi(x_1)\psi^*(x_2)\rangle$ and is called the density matrix — 'density' because $\langle|\psi(x)|^2\rangle$ is proportional to atom density and 'matrix' because it has two independent labels x_1 and x_2. This product of ψ evaluated at two different points is clearly related to the function inside the integral that defines the Wigner function in equation (7). If you carry out an average over possible pure-state Wigner functions you obtain $\langle W(x, P_x)\rangle$. This is, according to equation (7), the Fourier transform of the density matrix $\langle\psi(x+x'/2)\psi^*(x-x'/2)\rangle$. This is to say that by using quantum tomography on an atomic beam we can evaluate its important wave-coherence properties.

A laser is a device whose operation naturally creates coherent light, for which $\langle E(x_1)E^*(x_2)\rangle$ is large for large separations $|x_1-x_2|$ perpendicular to the beam-propagation direction. By analogy, a 'coherent atom-beam emitter' would create a coherent, high-density beam of atoms, for which $\langle\psi(x_1)\psi^*(x_2)\rangle$ is large over the full extent of the beam area. This means that essentially every atom is a part of the atomic group described by a single wave function $\psi(x)$, that is, $\langle\psi(x_1)\psi^*(x_2)\rangle\cong\psi(x_1)\psi^*(x_2)$.

Very recently the first source of coherent, high-density atoms in a beam-like geometry was demonstrated in the laboratory [30]. A high-density atomic gas was produced by cooling atoms in a magnetic trap to below the temperature needed for Bose–Einstein condensation (BEC) [31], at which point most of the atoms are in the ground-vibrational quantum state of the trap potential. Then the cold gas was launched out of the trap, producing a travelling pulse of coherent atoms. The pulse produced is similar in its coherence properties to the light pulse from a pulsed laser. But is not accurate to refer to the new device as an 'atom laser', as has been done, since there is no 'stimulated emission of atoms' here; atoms cannot be created and destroyed at low energies. Nevertheless, the creation of high-density beams of atoms might well prove to be as revolutionary for science as was the discovery of the laser in 1960. These ideas, and related ones, are discussed in articles by K. Burnett [32] and Adams [27] in *Contemporary Physics*.

It would be desirable to have a method to characterize fully the quantum state of a coherent atom-beam emitter. There is a serious barrier, though, to a straightforward application of quantum tomography for this purpose. In a high-density, low-temperature atom beam the atoms do not progagate independently of one another. They collide and interact cooperatively. This means that we can no longer assume free propagation in carrying out our analysis of the reconstruction problem. The presently known methods work only for low densities. Back to the drawing board!

8. Particle in an arbitrary potential — beyond the harmonic oscillator

So far I have discussed quantum motion corresponding to free-particle motion or motion in a harmonic potential. On the other hand, most motion is not so simple. For example, the vibration of a molecule that has been strongly excited is not well approximated by harmonic motion. Is it still possible to reconstruct its quantum state by observing its motion?

It turns out that due to special properties of the Schrödinger dynamical equation the answer to this question is yes. If you can measure the probability distribution Pr $(q;t)$ for particle position q at many different times t (ideally *all* times) then it is straightforward to reconstruct the state. This is done by using a generalized version of the Radon inversion transform, given earlier as equation (5). The details are given in [33].

9. Beyond the Radon-transformation method

It should be mentioned that recently improved mathematical methods have been developed that allow one to obtain the quantum state from the measured quantum-variable histograms without using the inverse Radon transformation. Using these methods the quantum state is found in the basis of the energy eigenstates, rather than in the position, or quadrature, basis which has been emphasized in this paper for simplicity. The new method is more robust against numerical problems and should be considered by anyone with a serious interest in this topic. Reviews of this approach can be found in [22] and in the works by Leonhardt and by D'Ariano listed in Suggestions for Further Reading.

10. Conclusions

I have tried to make the Schrödinger wave function a little less mysterious by showing that its form truly can be determined from a set of measurements on a collection of identically prepared particles or other physical systems. This should allow a firmer understanding of the meaning of ψ. I called it, along with its transformation rules, an

information structure. I like this name because it separates it from the idea of a physical field, such as the electric field. The name also makes it clear that the wave function is not the particle itself. This does not mean that the wave function represents information about a particle which has some definite but unknown values of momentum and position; rather it represents the maximum knowable information about how these quantities behave when they are 'measured,' according to John Bell [34].

None of these conclusions are essentially new to quantum mechanics, rather they only strengthen QM by making some of its basic hypotheses more concrete than had been possible in the past. So to me it seems that it has been worth doing.

We can return to the question—is the concept of wave function meaningful for a single particle? I believe that it is, but in a strange way. It should be clear from the discussion in this paper that if you are given only one particle out of a collection of many that have been prepared according to a certain procedure, you cannot measure the corresponding quantum state. You need the whole collection in order to carry out quantum tomography. It is also known that making repeated measurements on the same particle will not work to determine the state—this perturbs it and changes its state [35]. Nevertheless, it still does make sense to say that the particle has been prepared 'in' a certain quantum state, that is 'according to' a certain state-preparation procedure.

I seem to be forced to conclude that a single quantum particle is fundamentally incapable of carrying with it the full information about how it was prepared, or, if it does, it cannot yield up this full information to an observer. It seems that some information is lost or obscured, even for a pure state. In contrast, a large collection of identically prepared particles does carry sufficient information so that by a set of suitable measurements on a limited set of variables an experimenter can fully determine the state. Then the transformation rules allow him or her to predict with confidence, not the behaviour of any one particle, but the statistical behaviours of *all* of the properties of the group. This information is preserved and transmitted quite sharply. Such is the information structure that nature presents us with.

Acknowledgements

Suggestions for further reading

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[5] This definition of state is consistent with the 'Statistical Interpretation' of quantum mechanics as discussed by Ballentine, L. E., 1970, *Rev. Mod. Phys.*, **42,** 358; Newton, R. G., 1980, *Amer. J. Phys.*, **48,** 1029. This interpretation, in its strongest form, assumes that quantum mechanics is a theory only of the behaviour of macroscopic objects (eg. measuring devices) *and nothing more*. My use of the assumptions 1 – 3 does not imply that I take this strong interpretation literally.

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