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Abstract.   Quantum state diffusion provides a dynamics for the localization or reduction of a quantum-mechanical wavepacket during a measurement or similar physical process. The essence of this localization dynamics is captured in the classical theory presented here, which applies to the common situation where the localization takes place over macroscopic distances and the wave properties of the system are no longer relevant. It provides a picture of the localization process in classical phase space, and a practical aid for computations on open quantum systems. The theory is developed from classical Hamiltonian dynamics in phase space and the known properties of localization. As an example it is used to illustrate how absorption by a screen leads to quantum jumps. A derivation from quantum state diffusion using the Wigner function is given in the companion paper.

1. Introduction—density localization theory

Quantum state diffusion plays two distinct roles. One is in practical computations on open quantum systems [6–9] and the other is in providing a dynamics for the process of measurement, thus removing the need for a separate measurement hypothesis in quantum mechanics [10–16]. In both of these there is a clear need for a classical theory of localization.

Open quantum systems are important in many fields of physics, including quantum optics, noise in proposed quantum computers and energy transfer systems in molecular biology. Quantum state diffusion has proved its worth as a practical tool for computations on open quantum systems, and localization has proved to be a crucial property of the method, particularly when a moving basis is used [6, 7]. The classical theory of this paper provides a picture and a possible computational aid for numerical modelling of systems in which the total number of quantum basis states has to be large, yet ordinary classical mechanics cannot be applied. It can also be used as a means of making a preliminary investigation of the feasibility of a full quantum state diffusion computation, without a large initial commitment of computer time.

In quantum state diffusion and some other approaches to quantum theory, the reduction, collapse or localization of a wavefunction is a feature of a measurement, or similar interaction of a quantum system with its environment. In ordinary quantum theory the localization is not derived from the Schrödinger dynamics, but requires additional assumptions which are part of the interpretation of quantum theory. In quantum state diffusion theory (QSD) and similar theories, the localization is a dynamical process, requiring additional stochastic terms in the wave equation. Detailed references are given in the companion paper [1].

In measurement theory, the density diffusion provides a simpler picture of localization by measurement than QSD, in the common situations where the wave properties of the quantum states are no longer relevant.

In a Stern–Gerlach experiment, the two spin states of a beam of atoms are separated in space, and detected along two macroscopically distinct lines. The localization of each atom produced by the detection process is to one or other of these lines, and so takes place on a macroscopic scale. This is typical of quantum measurements, and suggests a classical localization theory, which is illustrated by the simplified example of absorption by a screen presented in section 9.

Hamiltonian dynamics can be derived as a classical limit of Schrödinger dynamics, but it is usually treated as an independent theory in its own right. Here we show that the essence of localization of quantum states in phase space can be treated similarly. It is captured in a classical picture, which is also introduced directly as an independent theory. Physical processes are easier to visualize in phase space than in Hilbert space. The properties of density localization are obtained from the known properties of localization dynamics in quantum state diffusion and similar theories. From these properties we obtain the basic density diffusion equations, which are the classical limit of the quantum state diffusion equations.

The classical theory of this paper was introduced and briefly discussed in [2]. The phase-space representation and the semiclassical expansion of the Wigner function in QSD are treated in detail in [1].

Quantum state diffusion is very different from ordinary classical Hamiltonian dynamics. There are two features in particular that distinguish them. One is that in QSD matter has wave properties, such as interference and diffraction, and the other is the property of localization. The Schrödinger equation captures the first, but not the second. The density localization theory introduced here captures the second but not the first. The relations between the theories are illustrated in figure 1.

For simplicity the density diffusion theory of this paper is restricted to nonrelativistic systems whose interactions with the environment are represented by Hermitian Lindblad
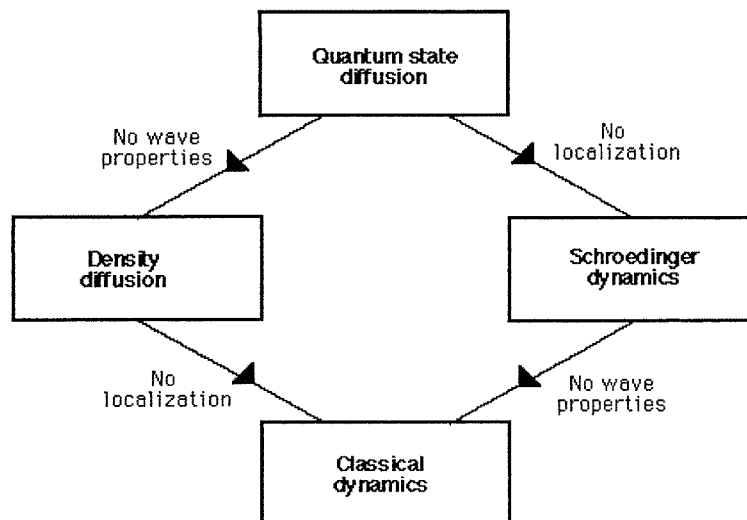

Figure 1. Relations between theories.

operators in QSD. These include interactions with measurement apparatus and similar interactions. In density diffusion theory they are represented by the corresponding Lindblad dynamical variables. For simplicity we exclude dissipative processes, such as interactions with a heat bath, that are represented by non-Hermitian Lindblad operators. For the same reason we do not give a detailed derivation of the density diffusion theory from QSD. Both of these are found in the companion paper [1].

Sections 2 and 3 introduce the basic properties of the densities of individual quantum systems, whilst section 4 deals with ensembles of such systems. A basic density diffusion equation is derived from some simple conditions in section 5, and it is generalized in section 6. The following two sections provide measures of localization, entropy in section 7 and variance in section 8. Section 9 applies the theory to localization of the particles of a beam that strikes a solid surface, providing a paradigm for quantum measurement, and showing how quantum jumps can be derived from this classical version of quantum state diffusion.

2. Classical systems and quantum densities

The state of a single classical system is represented by a point (q, p) in phase space, where q and p are vectors representing coordinate and conjugate momentum, each with d freedoms. A single quantum system without its wave properties is represented here by a *quantum density* $D(q, p)$, which is never negative.

The dynamics of a classical system is represented by a trajectory $(q(t), p(t))$ through phase space. For Hamiltonian dynamics with Hamiltonian $H(q, p, t)$, the trajectory is determined by Hamilton's equation

$$(\dot{q}, \dot{p}) = (\partial H / \partial p, -\partial H / \partial q). \tag{2.1}$$

The probability of a state of an ensemble in classical statistical mechanics is represented by an ensemble of points in phase space whose probability distribution is $\rho(q, p)$. When the system is isolated, so that there is no interaction with the environment, the value of $\rho(q(t), p(t))$ remains constant as the state moves along the trajectory following Hamilton's equations. We say that the phase point is carried by the Hamiltonian flow in the phase space. The time dependence of the distribution $\rho(q, p)$ as a function of fixed points (q, p) is given by the linear Liouville equation

$$\frac{\mathrm{d}\rho(q, p)}{\mathrm{d}t} = \frac{\partial \rho}{\partial q} \frac{\partial H}{\partial p} - \frac{\partial \rho}{\partial p} \frac{\partial H}{\partial q}. \tag{2.2}$$

Quantum systems are different. A single electron, neutron or atom can be in two or more places at once. This is clear from the evidence of two-slits and other interferometry experiments. A quantum system cannot therefore be represented by a point in phase space. However, a single quantum system in a pure state, but without its wave properties, can be represented by a non-negative normalized density $D(q, p)$ such that

$$\int_{\Omega} D(q, p, t) = 1 \tag{2.3}$$

where $\int_{\Omega}$ represents an integral over all phase space.

For quantum particles we have to work with both densities D and distributions ρ in phase space, and keep the distinction between them. For every density, dynamical variables have density expectations, variances and covariances, but these must not be confused with the corresponding quantities for the distributions. A density and a density expectation are quantum properties of the system, even though their representation is classical.

The density D is not a probability distribution like ρ, although when there is no localization it behaves like one. Quantum wave properties, such as interference and diffraction, are not represented whereas localization properties are.

The density D can be obtained from the Wigner distribution W by smearing it out over phase-space volumes much larger than $2\pi\hbar$, but we have here a different approach. W retains the wave properties, and shows structure on scales down to phase-space areas of $\hbar$ and below. It can be negative, whereas the density D is always positive. The quantum density D has none of the characteristic wave properties such as interference and diffraction, and shows structure only on larger scales. Just as in classical mechanics, phase-space regions whose size in any two-dimensional phase subspace is around $2\pi\hbar$ or less are treated like points. There are many types of phase-space distributions representing quantum systems, some of which are more smeared out than others. The density D is *very* smeared out.

In ordinary classical ray optics, where the scales are large compared with the wavelength of light, the light intensity is a course-grained average. The rays are like classical trajectories of particles moving in space. Ray optics is a good approximation on scales much larger than a wavelength, but does not provide any information about wave properties such as interference and diffraction.

The *quantum density* $D(q, p)$ in phase space is a course-grained average. Its dynamics is made up of ordinary Liouville dynamics, together with the dynamics of localization, which has no counterpart either in ordinary classical dynamics, or in classical ray optics. Like its optical analogue, the dynamics of quantum densities is a good approximation on scales much larger than a wavelength, but does not provide any information about quantum wave properties.

The loss of the wave properties provides a classical picture of the physics of quantum localization and also makes the analysis much simpler than for QSD . A particle in a beam can be represented by a density D that is spread throughout some volume of the beam, which is often of macroscopic dimensions. It is also spread in momentum. A free electron in a solid at room temperature is represented by a density D distributed within the solid. An electron in a beam which strikes the surface of the solid may be represented by a density that is partly in the beam, and partly in the solid, an important case for us, analysed in section 9.

A special density is the point density

$$D(q, p) = \delta(q - q_0, p - p_0) = \delta(q - q_0)\delta(p - p_0) \tag{2.4}$$

which represents a phase-space point on scales which are large compared with the Planck volume.

Without localization, the density $D(q, p, t)$ satisfies the same classical Liouville equation as the distribution $\rho(q, p, t)$ of the phase-space points of an ensemble of classical systems. Localization introduces additional stochastic localization terms. Point densities are already localized, so the localization has no effect on them, and they follow Hamiltonian trajectories in phase space. For sufficiently strong localization, densities localize so much that after a time they become indistinguishable from point densities, and then satisfy ordinary classical dynamics. This classical picture has the same strengths and weaknesses as ordinary classical dynamics. It no longer works on scales determined by Planck's constant, and does not represent the wave properties of material particles, which are treated in the companion paper [1].

Localization is a stochastic process, so the quantum density $D(q, p, t)$ satisfies a stochastic differential equation in time. The probability $\Pr(D)$ that there is a particular density D is represented by an ensemble of densities. This probability is a function of

points in density space. It is a large space, like the Hilbert space of quantum mechanics, but fortunately it is not used very much.

3. Quantum expectations and other properties of densities

The integrated value of D over a region α of phase space is a quantum weight, not a probability, although it is related to a probability through the stochastic dynamics of localization. Dynamical variables have expectations, given by averaging over the densities or weights.

For densities D, expectations, quantum variances and quantum covariances are defined just like the corresponding means, variances and covariances of classical probability distributions.

For density D, representing a pure quantum state, the weighted average of a dynamical variable B is the *expectation*

$$\langle B \rangle = \langle B \rangle_D = \int_\Omega D(q, p) B(q, p) \tag{3.1}$$

where $\int_\Omega$ represents the integral over the entire phase space. The simplest example is the norm $N(D)$ of D, which is the expectation of unity,

$$N(D) = \langle 1 \rangle = \int_\Omega D(q, p) \cdot 1.$$

For D to be the classical representation of a pure quantum state, the norm must always be unity.

The square of the variation of B around the expectation $\langle B \rangle$ is the quantum *variance*

$$\sigma^2(B) = \sigma(B, B) = \langle (B - \langle B \rangle)^2 \rangle = \langle B^2 \rangle - \langle B \rangle^2 \tag{3.2}$$

which is used in sections 5 and 8.

The ensemble localization $\Lambda(B)$ of B is defined to be the inverse of the mean over the ensemble of the quantum variance of B:

$$\Lambda(B) = 1/M\sigma^2(B). \tag{3.3}$$

The quantum *covariance* of two dynamical variables B and C is

$$\sigma(B, C) = \langle (B - \langle B \rangle)(C - \langle C \rangle) \rangle = \langle BC \rangle - \langle B \rangle \langle C \rangle. \tag{3.4}$$

For ordinary classical probability distributions, the covariance is a measure of the correlation of B and C, but for these densities it is a measure of the quantum *entanglement* of B and C. Because of localization, the properties of entanglement are essentially different from the properties of correlation. In fact it is primarily this property of entanglement that makes quantum systems behave so strangely. Our use of 'entanglement' here is a generalization of its normal use in quantum mechanics.

The density dispersion entropy S_D of a density D is minus the mean of the logarithm of the density:

$$S_D = -\langle \ln D \rangle = -\int_\Omega D(q, p) \ln D(q, p). \tag{3.5}$$

It is a useful logarithmic measure of the dispersion of the density D in phase space. The more the density is dispersed throughout the space, the larger the entropy. The faster the density localizes in phase space, the faster the entropy decreases, as shown in section 7.

The quantum dispersion entropy of [3] depends on a partition of the state space into channels, but the density dispersion entropy is independent of any such partitions.

4. Probability distributions and means

Like phase space points for open classical systems, phase space densities for open quantum systems obey statistical laws. A quantum system which interacts with measuring apparatus is open, and it is this type of interaction which concerns us.

   Localization is a stochastic process. Given a single initial density D, the future densities cannot be predicted exactly, but they have a probability distribution $\Pr(D)$ defined over the large space of all densities D. The distribution ρ is defined in terms of the probabilities $\Pr(D)$. If there is only one density $D(q, p)$ in the ensemble, then $\rho(q, p) = D(q, p)$. When there is more than one density, then ρ is an ensemble mean over densities:

$$\rho(q, p) = \int_D \Pr(D)D(q, p) = \mathrm{M}D(q, p) \tag{4.1}$$

where the integral in the space of densities is always taken over all densities D. If the probability distribution ρ is derived from the distribution of densities $\mathrm{P}(D)$, then the ensemble mean of the expectation for a dynamical variable B is

$$\mathrm{M}B = \mathrm{M}\langle B \rangle = \int_D \Pr(D)\langle B \rangle = \int_D \Pr(D)\int_\Omega D(q, p)B(q, p). \tag{4.2}$$

   This will be called the ensemble mean, or even just 'the mean' of B. Unlike the expectation for a pure state it is a property of ensembles. In the special case when the only significant densities D are point densities, then ρ is the usual phase space distribution of phase points for the particles, and the ensemble mean is the usual ensemble mean of classical statistical mechanics. We will show that the dynamics of localization tends to make systems approach this special case.

   This mean is linear in D. However, we will be particularly interested in the means of variances, like $\mathrm{M}\sigma^2(B)$, because they can be used to measure the mean localization for an ensemble of densities. These are quadratic in D. Quadratics in D also appear in the localization dynamics of densities, which is therefore nonlinear, unlike the Liouville equation (2.2).

   For quantum particles we have to work with both quantum densities and distributions in phase space, and keep the distinction between them. The quantum density expectations, variances and covariances must not be confused with the corresponding quantities for the distributions. The quantum expectation and variance, like the density itself, is a quantum property of the system, even though its representation is classical.

5. Diffusion of quantum densities

At first, suppose that the diffusion depends on a single dynamical variable L, corresponding to a Hermitian Lindblad operator in QSD. This represents the localization of a dynamical variable cL, where c is a nonzero constant. There are many processes which can produce such localization, including the measurement of a dynamical variable cL. The localization for a given density D increases as the variance $\sigma^2(L)$ decreases. The ensemble localization $\Lambda(B)$ is a direct measure of localization for the whole ensemble. When it increases, we can say with confidence that localization is taking place.

   The fundamental quantum density diffusion equations which localize the densities need to satisfy a number of reasonable conditions. The simplest possible linear equation satisfies all the conditions except the normalization condition, which can easily be retained by introducing a quadratic normalization term. A number of important results follow.

   The first two are conditions on the density D itself. They are

(Co1) the norm $N(D)$ of D is conserved;

(Co2) the non-negativity of D is preserved.

The rest are conditions on the mean, variance and localization of dynamical variables, when the localization is controlled by a single 'Lindblad' dynamical variable $L(q, p)$. Their choice is guided by the properties of dynamical variables in QSD. The dynamical variable $B(q, p)$ is arbitrary.

(Co3) The ensemble mean of any B remains constant.

(Co4) The dynamical variable cL localizes for all real nonzero c.

The only condition that may be surprising is (Co3), which is not true for QSD. However, in QSD, only dynamical variables which do not commute with L change their mean values, and in the classical limit of density diffusion theory the commutator goes to zero.

To obtain the density diffusion equations, first assume for simplicity an initial ensemble at time t with only one density $D(t)$. At later times the ensemble will have many densities.

Because of (Co2), $D(t)$ is real for all times, so the fluctuations must be real. Real fluctuations are denoted $dw = dw(t)$, where

$$M dw(t) = 0 \qquad M(dw(t))^2 = dt \qquad M(dw(s) dw(t)) = 0 \qquad (s \neq t). \qquad (5.1)$$

Let M be the mean over these fluctuations, as usual. The simplest nontrivial diffusion equation for a density D which includes the Lindblad dynamical variable L and the fluctuation dw is

$$dD = LD dw \qquad \text{(trial equation).} \qquad (5.2)$$

This equation is linear in D, but it cannot be correct, because the norm is not conserved:

$$dN(D) = \langle L \rangle dw. \qquad (5.3)$$

This can be rectified by subtracting the expectation of $\langle L \rangle$ from L, giving

$$dD = (L - \langle L \rangle) D dw. \qquad (5.4)$$

This is the simplest density diffusion equation. $\langle L \rangle$ is linear in D, so the right-hand side of the evolution equation is quadratic in D, and because it is nonlinear, the density $D(q, p)$ cannot be a probability distribution. The expectation $\langle L \rangle$ depends on the value of $D(q, p)$ in all regions of phase space for which it is not zero. So the change in D depends on its value in all these regions. This usually means that the evolution is nonlocal, as quantum localization is known to be.

So this density diffusion equation is nonlinear in D and nonlocal.

We now demonstrate that the solution of (5.4) satisfies all the conditions (Co1)–(Co4). For the normalization condition (Co1),

$$dN = d \int_\Omega 1 \cdot dD = \int_\Omega (L - \langle L \rangle) D dw$$
$$= \langle (L - \langle L \rangle) \rangle dw = 0. \qquad (5.5)$$

For (Co2), if the value of $D(q, p)$ at any point (q, p) is zero, then it remains unchanged, so by continuity D cannot pass the value zero.

For (Co3), the change in the expectation of an arbitrary dynamical variable B is

$$d\langle B \rangle = \int_\Omega B dD$$
$$= \int_\Omega (B(L - \langle L \rangle)) D dw = \langle (B(L - \langle L \rangle)) \rangle dw$$
$$= \sigma(B, L) dw \qquad (5.6)$$

so for arbitrary B,

$$M\,d\langle B\rangle = 0 \tag{5.7}$$

which confirms (Co3).

For (Co4), we need particular cases of (5.6) and (5.7) for $B = L$ and $B = L^2$. These are

$$d\langle L\rangle = \sigma^2(L)\,dw \qquad M\,d\langle L^2\rangle = 0. \tag{5.8}$$

We also need the Itô differential of a product, which is

$$d(xy) = dx \cdot y + x\,dy + dx \cdot dy \tag{5.9}$$

so the ensemble mean of the change in the variance of L is

$$\begin{aligned} M\,d\sigma^2(L) &= M\,d\langle L^2\rangle - M\,d(\langle L\rangle^2) \\ &= -M((d\langle L\rangle)^2) \\ &= -M(\sigma^2(L)^2)\,dt \end{aligned} \tag{5.10}$$

from equation (5.8).

So the mean of the quantum variance of L decreases unless it is already zero, and the same applies to cL for nonzero c. A Lindblad dynamical variable L of density diffusion theory is itself localized.

It also localizes any dynamical variable B for which the covariance $\sigma(B, L)$ is not zero. From equation (5.6), for arbitrary B,

$$M\,d\sigma^2(B) = -M(\langle B\rangle)^2 = -[\sigma(B, L)]^2\,dt \tag{5.11}$$

from which the result follows. So L deserves the name of 'localizer'.

6. Generalization

A general density diffusion equation has a Hamiltonian H and many localizers L_j with their corresponding fluctuations dw_j:

$$dD = \{D, H\} + \sum_j (L_j - \langle L_j\rangle)D\,dw_j \tag{6.1}$$

where $\{D, H\}$ is the usual Poisson bracket, and the fluctuations dw_j are independent and normalized to dt so that

$$M\,dw_j = 0 \qquad M\,dw_j\,dw_k = \delta_{jk}\,dt. \tag{6.2}$$

These orthonormal fluctuations dw_j are not unique. Any orthogonal transformation gives an equivalent set of orthonormal fluctuations $dw_j = \sum_k O_{jk}\,dw_k'$. It is useful to think of these as the *same* vector fluctuation in the fluctuation space, but in a different representation.

The localizers L_j may also be considered as a vector, in the space of dynamical variables. The orthogonal transformation $L_j = \sum_k L_k'(O^{-1})_{kj}$ gives a new set of localizers, and it follows that the equation

$$dD = \{D, H\}\,dt + \sum_k (L_k' - \langle L_k'\rangle)D\,dw_k' \tag{6.3}$$

is the same equation as (6.1). To preserve the density diffusion equations, an orthogonal transformation of the fluctuations must be complemented by an inverse orthogonal transformation of the localizers L_j. Since dw_k' is just a set of orthonormalized differential

fluctuations, they could be replaced by the original dw_k, which shows that the density diffusion equations are independent of the representation in L-space.

In particular, if the L_j are n linearly dependent localizers, with an m-dimensional space of linearly independent L, then there is an orthogonal transformation to a representation in which $n - m$ of them are zero and the remaining m of the L_j are independent. The zeros can be ignored so we can always assume that the localizers are linearly independent.

The density diffusion equations are invariant under orthogonal transformations in the localizer space. Any L' of the form $L' = \sum c_j L_j$ with $\sum_j |c_j|^2 = 1$ can be considered as one of the localizers, as in section 8. So equation (6.1) with linearly independent localizers is the general density diffusion equation.

See [1] for a derivation of (6.1) from the QSD equations, and [4] for the corresponding transformation theory for QSD.

In the laboratory the density of a particle such as an electron may be partly in a vacuum and partly absorbed in one of a number of solid objects. We can suppose that the vacuum and the objects divide position space into regions α. Frequently the form of the density within each region is of no importance, we are only interested in the weight for each region, given by integrating the position-space density over the whole region. For simplicity we suppose that the localization variable L in each region is uniform.

The phase-space theory is just as simple and more general, so we derive the diffusion equations for the discrete set of weights W_α given by integrating a phase-space density D over regions α,

$$W_\alpha = \int_\Omega P_\alpha D \tag{6.4}$$

where P_α is the characteristic function or projector which is 1 inside and 0 outside the region α. We deliberately choose a notation that highlights the parallel with the corresponding theory for projectors in QSD, which is treated in [3]. The expectation of the projector is

$$\langle P_\alpha \rangle = \int_\Omega D P_\alpha = W_\alpha. \tag{6.5}$$

As before we start with the simplest case of a wide open system with a single localizer

$$L = \sum_\alpha \ell_\alpha P_\alpha \tag{6.6}$$

whose expectation is

$$\langle L \rangle = \sum_\alpha \ell_\alpha W_\alpha \tag{6.7}$$

giving the density diffusion equation

$$dD = (L - \langle L \rangle) D \, dw. \tag{6.8}$$

The change of the weight dW_α is then

$$dW_\alpha = \int_\Omega P_\alpha \, dD = \int_\Omega P_\alpha (L - \langle L \rangle) D \, dw = (\ell_\alpha - \sum_\beta \ell_\beta W_\beta) W_\alpha \, dw$$

$$= (\ell_\alpha - \langle \ell \rangle) W_\alpha \, dw \tag{6.9}$$

where by definition

$$\langle \ell \rangle = \langle L \rangle = \sum_\beta \ell_\beta W_\beta. \tag{6.10}$$

The equations generalize directly to the case of many localizers L_j as

$$dW_\alpha = \sum_j (\ell_{j,\alpha} - \langle \ell_j \rangle) W_\alpha \, dw_j \qquad (6.11)$$

which is the stochastic diffusion equation for the weights.

The special case of one localizer for each region applies, for example, to the case of position-space localization. In that case we can label the localizers with α. They are

$$L_\alpha = \ell_\alpha P_\alpha \qquad \text{so} \qquad \ell_{j,\alpha} = \delta_{j\alpha} \ell_\alpha \qquad (6.12)$$

and the density diffusion equations become

$$dW_\alpha = \left(\ell_\alpha \, dw_\alpha - \sum_\beta \langle \ell_\beta \rangle \, dw_\beta \right) W_\alpha. \qquad (6.13)$$

Note that the Hamiltonian evolution has not been included in this generalization. A particular case with Hamiltonian evolution included is given in section 9.

7. Density entropy decreases

Entropy is a natural measure for the spread of a probability distribution ρ of classical systems in phase space. It can be used similarly to measure the spread of the quantum density D.

The entropy S_D of a density D is defined as

$$S_D = - \int_\Omega D \ln D. \qquad (7.1)$$

To obtain changes in S_D with time, we need changes in the integrand, which requires the expansion of $\ln D$ up to second order in D. It is given by

$$d(D \ln D) = dD \cdot (1 + \ln D) + (dD)^2/(2D). \qquad (7.2)$$

Using this and $M dD = 0$, we have, using the orthonormality of the fluctuations, that

$$M \, dS_D = - \int_\Omega (dD)^2/(2D) = -\tfrac{1}{2} \int_\Omega \sum_j (L_j - \langle L_j \rangle)^2 D = -\tfrac{1}{2} \sum_j \sigma^2(L_j). \qquad (7.3)$$

We can think of $\sum_j \sigma^2(L_j)$ as the variance of the vector localizer $L = \{L_j\}$.

The Hamiltonian evolution does not change the density along the classical paths, so it makes no contribution to the change in the entropy of the density. So unless the variances are all zero, and the density is confined to a subspace of the phase space in which all the L_j are constant, the entropy of the density always *decreases*. This is the density entropy theorem.

Since localization tends to concentrate the density in the phase space, it is not surprising that the entropy always decreases as a result of the localization. This is in contrast to the usual idea as to how an entropy should behave. It is one of the remarkable properties of the observed localization of matter in a quantum measurement.

Since the probability distribution ρ remains constant along the Hamiltonian trajectories, the distribution entropy

$$S = - \int_\Omega \rho \ln \rho \qquad (7.4)$$

remains constant. We cannot use the decrease in entropy to gain useful work, because the loss of entropy of the densities for each member of the ensemble is cancelled by the increase

in the distribution entropy which results from the fluctuations. The net result is a constant distribution entropy S. If there is a dissipative interaction with the environment, which we do not consider here, the distribution entropy does not remain constant, but increases.

The second law of thermodynamics is about ρ, not about D, and is not violated by the theorem. No experimenter nor engineer can predict the values of the random variables $\mathrm{d}w(t)$, and so they cannot predict which of the densities D of the ensemble is going to appear. Without this knowledge it is not possible to take advantage of the decrease in entropy of the densities of pure states.

For chaotic systems with weak localization, the entropy density theorem can be deceptive. According to the theorem, the regions of phase space in which the density is large decrease in volume, but according to chaos theory, they become stretched, folded and squeezed. The result can be that the regions of high density become small, but dispersed over much of the chaotic region.

It is for this reason that in the next section, the localization theorem is for wide open systems, in which the effect of the Hamiltonian is negligible.

8. Localization for wide open systems

In wide open systems the effect of the Hamiltonian is negligible in comparison with the effect of the localizers. The theory of wide open systems is more useful than one might expect, since interaction representation can often be used to remove the effect of the Hamiltonian.

Suppose that there are many L_j, and let B, B' be arbitrary dynamical variables, not necessarily connected with the L_j in any way. By using the same methods as in section 5, it is easy to show that conditions (Co1)–(Co3) are satisfied for wide open systems when there are many localizers.

For (Co4) it is slightly more complicated. For an arbitrary B,

$$\mathrm{d}\langle B\rangle = \int_\Omega \sum_j (B(L_j - \langle L_j\rangle))\,\mathrm{d}w_j = \sum_j \sigma(B, L_j)\,\mathrm{d}w_j. \tag{8.1}$$

The mean change in the covariance of B, B' is

$$\mathrm{M}\,\mathrm{d}\sigma(B, B') = -\mathrm{M}\,\mathrm{d}\langle B\rangle\,\mathrm{d}\langle B'\rangle = -\mathrm{M}\sum_{jk} \sigma(B, L_j)\,\mathrm{d}w_j\,\sigma(B, L_k)\,\mathrm{d}w_k$$

$$= -\mathrm{M}\sum_j \sigma(B, L_j)\sigma(B', L_j)\,\mathrm{d}t. \tag{8.2}$$

Two special cases of this result are particularly useful. When $B = B'$,

$$\mathrm{M}\,\mathrm{d}\sigma^2(B) = -\mathrm{M}\sum_j [(\sigma(B, L_j)]^2\,\mathrm{d}t \tag{8.3}$$

which is minus a sum of squares. Any dynamical variable therefore localizes, unless its covariance with *all* the localizers is zero.

Specializing further, suppose L' is a localizer, and $B = B' = L'$. In a basis in which $L' = L_1$, we have

$$\mathrm{M}\,\mathrm{d}\sigma^2(L') = -\mathrm{M}\sum_j \sigma(L_1, L_j)^2\,\mathrm{d}t \leqslant -(\mathrm{M}\sigma^2(L'))^2\,\mathrm{d}t. \tag{8.4}$$

Now suppose that X is any quantity defined for each member of the ensemble. The *ensemble* variance $\Sigma^2(X)$ is never negative, so

$$0 \leqslant \Sigma^2(X) = \mathrm{M}(X^2) - (\mathrm{M}X)^2 \qquad -\mathrm{M}X^2 \leqslant -(\mathrm{M}X)^2. \tag{8.5}$$

Putting $X = \sigma^2(L')$ we obtain

$$d(M\sigma^2(L')) = M\,d\sigma^2(L') \leqslant -M(\sigma^2(L'))^2\,dt \leqslant -(M\sigma^2(L'))^2\,dt. \qquad (8.6)$$

The ensemble localization of L' is defined in (3.3) as the mean of the inverse of the variance, so

$$d\Lambda^{-1}/dt \leqslant -\Lambda^2 \qquad d\Lambda/dt \geqslant 1 \qquad\qquad (8.7)$$

and the localization of a localizer increases linearly with time t or faster. There is a similar result for any dynamical variable in the localizer space, with a possible external positive constant.

When the localization increases, the variance decreases. Unlike the entropy of the density, for a system that is open but not wide open, the variance of a dynamical variable can be increased as a result of the Hamiltonian evolution. For example, a density D of a free particle with a spread of momentum and no localizer has a position variance that increases linearly with time. In chaotic systems variances increase exponentially.

So for systems with nonzero Hamiltonians and localizers there is often competition between them. When the localization is sufficiently strong, the density localizes to a small region around a phase point which then moves in phase space like the phase point of the simple Hamiltonian system. When the localization is very weak, the result depends on the Hamiltonian. Except for special cases, for example when there is a single localizer, which is conserved by the Hamiltonian, integrable systems localize. Chaotic systems were discussed above and in section 7.

9. Localization of a particle in a medium

The system of this section has also been treated using QSD and projection operators in [5].

The medium can be a solid, liquid, gas or vacuum. The particle is the system and the medium is the environment, which is treated as uniform, so the rate of localization is independent of the position of the particle within it. For the vacuum it is supposed to be zero. For many different media, each medium occupies a volume labelled α, which includes the whole of the momentum space and a restricted part of position space. The theory of section 6 can be used, in which the localization into different regions is expressed in terms of weights W_α. The localization rate can depend on the momentum of the particle, but for simplicity we will neglect this dependence, so the momentum dependence of the distribution plays no role, and we can use densities $D(r)$, regions α, and the corresponding weights W_α that depend on the three-dimensional position r alone.

The more interesting cases are those for which the system is not wide open, and the Hamiltonian has a significant effect. This holds for laboratory measurement of the properties of quantum systems, that is, quantum measurement. The principle is illustrated by a truncated uniform beam of unit length and velocity, containing a single particle with unit density ρ_0. The beam strikes a solid surface at time $t = 0$, which absorbs and localizes it in unit time. The distribution ρ for the ensemble is sketched in figure 2. We want to find the properties of the weights W_α whose means are probabilities P_α. The statistical properties are represented by an ensemble of such systems. The density D_0 of each particle of the ensemble is uniform before it strikes the surface, but unlike ρ_0 it is not unity, because of the localization. Suppose the regions of position space are labelled by $\alpha = 0$ for the vacuum and $\alpha = 1$ for the solid.
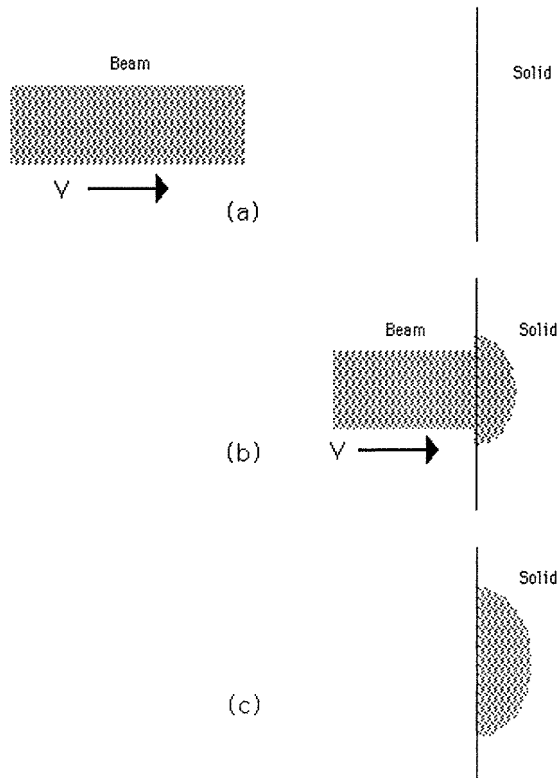
Figure 2. Truncated one-particle beam striking a solid surface. The hatched regions sketch the distribution ρ (*a*) before, (*b*) during, and (*c*) after entry.

All integrals $\int$ are integrals over position space, so the ensemble probabilities P and the individual particle weights W_α are

$$P_0 = \int_{\text{beam}} \rho = 1 - t \qquad W_0 = \int_{\text{beam}} D$$

$$P_1 = \int_{\text{solid}} \rho = t \qquad W_1 = \int_{\text{solid}} D \tag{9.1}$$

with the properties

$$\text{M}W_\alpha = P_\alpha \qquad \sum_\alpha W_\alpha = \sum_\alpha P_\alpha = 1. \tag{9.2}$$

Because of localization, the weight W_0 may be greater or less than P_0. The density D_0 does not change as a result of the Hamiltonian dynamics, but the length of the beam is $1 - t$, so

$$\mathrm{d}W_0 = -D_0 \, \mathrm{d}t \qquad \text{(Hamiltonian)}. \tag{9.3}$$

W_1 increases at the same rate.

We will show that the weights are nearly always close to 0 and 1, and change suddenly from one to the other. That is, that the weights change in jumps. The dispersion of the weights W_0 and W_1 is conveniently measured by the quantum variance of α, that is

$$\sigma^2(\alpha) = \langle \alpha^2 \rangle - \langle \alpha \rangle^2 = W_1 - W_1^2 = W_1 W_0. \tag{9.4}$$

This is small for strong localization, when the weights are close to 0 or 1, larger otherwise. Before $t = 0$ and after $t = T$ the quantum variance $\sigma^2(\alpha)$ is zero. We now show that its ensemble mean is very small at all times.

Since the density diffusion is uniform in the solid, it can be represented by

$$
\begin{aligned}
L(r) &= \ell_1 && \text{(solid)} \\
L(r) &= 0 && \text{(beam), so} \\
\langle L \rangle &= \ell_1 W_1
\end{aligned}
\tag{9.5}
$$

where ℓ_1^2 is a rate which is determined by interactions of the particle within the solid, and is therefore very fast in comparison with macroscopic rates.

From equations (6.11) and (9.5), the change in W_0 due to density diffusion in the solid is therefore

$$
\mathrm{d}W_0 = -\langle L \rangle W_0 \, \mathrm{d}w = -\ell_1 \sigma^2(\alpha) \, \mathrm{d}w \qquad \text{(diffusion).}
\tag{9.6}
$$

Adding the Hamiltonian and diffusion contributions we get

$$
\mathrm{d}W_0 = -D_0 \, \mathrm{d}t - \ell_1 \sigma^2(\alpha) \, \mathrm{d}w.
\tag{9.7}
$$

Because of the normalization condition in (9.2) there is no need for a separate equation for W_1.

The change in the mean quantum variance of α is

$$
\begin{aligned}
\mathrm{M}\,\mathrm{d}\sigma^2(\alpha) &= \mathrm{M}[(1 - 2W_0)\,\mathrm{d}W_0 - (\mathrm{d}W_0)^2] \\
&= \mathrm{M}(2W_0 - 1)D_0 \, \mathrm{d}t - \ell_1^2 \mathrm{M}[\sigma^2(\alpha)]^2 \, \mathrm{d}t \\
&\leqslant \mathrm{M}D_0 \, \mathrm{d}t - \ell_1^2 \mathrm{M}[\sigma^2(\alpha)]^2 \, \mathrm{d}t \qquad (W_0 \leqslant 1) \\
&= \mathrm{d}t - \ell_1^2 \mathrm{M}[\sigma^2(\alpha)]^2 \, \mathrm{d}t \qquad (\mathrm{M}D_0 = 1).
\end{aligned}
\tag{9.8}
$$

The first Hamiltonian term increases the mean variance, and the second density diffusion term tends to decrease it. Replacing the inequality by an equality gives the boundary, which is obtained analytically, giving

$$
\begin{aligned}
\mathrm{M}\frac{\mathrm{d}\sigma^2(\alpha)}{\mathrm{d}t} &\leqslant \ell^{-1} \frac{1 - \mathrm{e}^{-2\ell_1 t}}{1 + \mathrm{e}^{-2\ell_1 t}} \\
&< \ell^{-1}.
\end{aligned}
\tag{9.9}
$$

Since ℓ_1^2 is a rate determined by the interactions of the particles within the solid, which is much faster than the rate at which the beam enters the solid, σ^2 is always much less than unity. So W_0 is nearly always very close to 1, its value at $t = 0$, or to 0, its value at $t = T$. Thus it must change very quickly, a good approximation to an instantaneous jump.

For a single system of the ensemble, the particle remains in the beam and then jumps suddenly into the solid. This is what happens when a quantum particle with an extended matter wave strikes a solid surface, which is justified by a verbal argument in the usual interpretation of quantum mechanics. Here it is derived from the dynamics of density diffusion, as an approximation to quantum state diffusion.

This theory applies generally to systems in which the interaction of the particle with a medium or measuring apparatus is fast, for example in a measurement of a state of a quantum system. This shows by means of a simple example how the quantum jumps which appear in quantum measurements can be derived from quantum-density diffusion. It is also an example of localization for which the wave properties of the quantum system are unimportant.

10. Discussion

Quantum systems appear to spread out like waves and then become localized like particles. In quantum state diffusion the localization is a stochastic physical process in which the states of individual quantum systems obey a nonlinear QSD equation and the state of an ensemble of quantum systems obeys a linear master equation. The quantum systems of QSD have both wave and localization properties. In this picture a Schrödinger equation is an approximation to a QSD equation in which the localization is neglected. It is a good approximation when the quantum system has a negligible effect on classical systems, but not during measurement, or for similar processes.

The density diffusion theory of this paper is an approximation to QSD in which the wave properties are neglected. It is a good approximation when the quantum system is interacting so strongly with its environment that its coherence no longer has any significant effect and its wave properties are almost completely lost. Such strong interactions occur when simple quantum systems interact with complicated systems such as solids, liquids and gases. They also occur when signals from quantum systems are amplified and when they are recorded, as in the formation of a photographic image [5]. They may also result from interaction of a quantum system with a heat bath.

In density diffusion the state of a quantum system is represented by a density in phase space, with a nontrivial combination of Hamiltonian and localization processes. This is a new kind of nonlinear classical dynamics whose properties are not yet fully worked out.

Usually localization depends on momentum as well as position, but where the dependence on momentum is relatively unimportant, the process of localization can be visualized in ordinary position space, as in the example of a particle in a beam striking a solid surface presented in section 9.

Density diffusion theory provides a new theoretical tool for the study of the dynamics of localization in quantum systems, and its relative simplicity opens up the possibility of studying more complicated or more subtle localization processes where the wave properties of Schrödinger dynamics and QSD may not be important.

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