

Unravellings

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References (This note relies heavily on [5] and [10]) /:

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1 The Master Equation

We have the Kraus representation theorem

$$\hat{\rho}_{\text{after}} = \sum_j \hat{E}_j \hat{\rho}_{\text{before}} \hat{E}_j^\dagger \quad (1)$$

with

$$\sum_k \hat{E}_k^\dagger \hat{E}_k \quad (2)$$

which guarentees that $\hat{\rho}_{\text{after}}$ satisfies the requirements of a density operator if $\hat{\rho}_{\text{before}}$ does.

Now let us suppose that $\hat{\rho}_{\text{before}} = \hat{\rho}(t)$ the density matrix at time t and that $\hat{\rho}_{\text{after}} = \hat{\rho}(t + dt)$ the density matrix at time $t + dt$. Equations 1 and 2 tell us how $\hat{\rho}(t + dt)$ and $\hat{\rho}(t)$ must be related, though we don't know what the \hat{E}_k operators are. However, *if* we assume that $\hat{\rho}(t)$ satisfies a first order differential equation¹, then one Kraus operator is $\mathbf{1} + \mathcal{O}(dt)$, and all the others are $\mathcal{O}(\sqrt{dt})$. Let us therefore write, with \hat{H} and \hat{K} both Hermitian

$$\begin{aligned} \hat{E}_0 &= \mathbf{1} + (-i\hat{H} + \hat{K})dt \\ \hat{E}_k &= \sqrt{dt}\hat{L}_j \quad j = 1 \dots \end{aligned} \quad (3)$$

¹This is, in essence, the Markov approximation, which says that the environment retains no memory which can return to haunt the system later.

and use equation 2, dropping terms higher than first order in dt , to get

$$\frac{d}{dt} \hat{\rho} = -i[\hat{H}, \hat{\rho}] + \sum_j \left(\hat{L}_j \hat{\rho} \hat{L}_j^\dagger - \frac{1}{2} \hat{L}_j^\dagger \hat{L}_j \hat{\rho} - \frac{1}{2} \hat{\rho} \hat{L}_j^\dagger \hat{L}_j \right), \quad (4)$$

where \hat{H} is the system Hamiltonian. The \hat{L}_j are called Lindblad operators, after G Lindblad, who proved equation 4 from the axioms of dynamical groups. The Lindblad operators represent the interaction of the system with the environment. Equation 4 is called the master equation.

2 Unravelling the master equation

We could write equation 4 as

$$\frac{d}{dt} \hat{\rho} = -i \left[\hat{H}_{\text{eff}}, \hat{\rho} - \hat{\rho} \hat{H}_{\text{eff}}^\dagger \right] + \sum_j \left(\hat{L}_j \hat{\rho} \hat{L}_j^\dagger \right) \quad (5)$$

where we use the effective, *non*-Hermitian Hamiltonian

$$\hat{H}_{\text{eff}} = \hat{H} - \frac{i}{2} \sum_j \hat{L}_j^\dagger \hat{L}_j \quad (6)$$

and the expression $\left[\hat{H}_{\text{eff}}, \hat{\rho} - \hat{\rho} \hat{H}_{\text{eff}}^\dagger \right]$ is the generalization of the commutator.

Now, there are several suggestive points to make:

1. If the last term in equation 5 — the ‘sandwich term’ — is ignored, then $\hat{\rho}$ could be derived from a Schrödinger equation

$$i \frac{d}{dt} |\Psi\rangle = \hat{H}_{\text{eff}} |\Psi\rangle \quad (7)$$

2. However, equation 7 does not preserve the normalization of $|\Psi\rangle$ ($\langle\Psi|\Psi\rangle$ shrinks). Since the master equation preserves normalization, we see that the last term is important for normalization and must be included.
3. If we persist in trying to find a wavefunction to represent the master equation, then equation 3 suggests that in a time interval dt the contribution to this wavefunction from the sandwich term scales as \sqrt{dt} !
4. Many stochastic processes are characterized by a \sqrt{t} time development, and, furthermore, the coupling between the system and environment, which started all this in the first place is supposed to be stochastic.

Thus, we may speculate that an ensemble of *stochastic* wavefunctions will be needed to represent the master equation’s density operator so that we have

$$\hat{\rho} = \sum_n s_n |\Psi\rangle_n \langle\Psi| \quad (8)$$

where s_n is the weight of the the wavefunction $|\Psi\rangle_n$ in the ensemble, and the subscript n labels the member of the ensemble. In the next section I discuss how to construct suitable stochastic wavefunctions; first, an interlude on why we might want to.

2.1 A practical example

Much of the course so far has concentrated on ‘small’ systems with ‘simple’ time developments. However, consider the problem of modelling the laser control of chemical reactions. Laser isotope separation of ^{235}U falls into this category and provides a useful illustration. One scheme requires the use of pulsed lasers to ionize ^{235}U through a ladder of three excited states. The object is to choose laser pulse shapes *etc* to optimize this excitation. Thus, the time development of the system, contained in \hat{H} , is important. However, the environmental influences which come from laser noise, collisions with other atoms *etc* must also be included. These are, of course, modelled by Lindblad operators.

An N level system has $N^2 - 1$ independent real components for its density matrix, but $2N - 1$ independent real components for its wavefunction. Thus, if only three levels were involved, then the density operator would require 8 real function of time; a wavefunction would require 5. This difference is not very significant. However, the ^{235}U nucleus has a spin of $7/2$, and the 3 levels each have an angular momentum ~ 6 . Thus, the ‘3’ level system actually involves ~ 312 quantum states. Now the density matrix needs the solution of 97343 coupled differential equations, whereas the wavefunction requires only 623. The difference now is clearly significant a significance which is exaggerated when we remember that the difficulty of solving a set of N differential equations scales roughly as N^3 . Thus, in this case it is $\sim 3.8 \times 10^6$ more difficult to solve for the density operator than to solve for a wavefunction. Crudely, we could perform the average implicit in equation 8 with ~ 4 million realizations, or equation 4 once with the same resources. Although this is an overestimate — it takes no account of symmetries and selection rules, which can reduce the number of coupled equations which need to be solved — it suggests that for large systems many (stochastic) Schrödinger equations can be solved for the price of one master equation.

2.2 Quantum fundamentals

There is a viewpoint which claims that the wavefunction is more ‘fundamental’ than the density operator, and that equation 4 is a calculational device to simplify the instruction ‘calculate the wavefunction for the whole system+environment; evaluate the expectation value of your observable with this wavefunction as a function of *all* the parameters needed to specify the wavefunction and finally average over the unobserved parameters’. Another viewpoint claims that the density operator is fundamental; equation 4 is the ultimate truth — we arrived at it by considering wavefunctions, and, under certain circumstances can still use wavefunctions to calculate $\hat{\rho}$, but generally we can’t. Quantum unravellings provide a third alternative. They enable us to calculate a ‘wavefunction’ for the system only, though with the disadvantage that this wavefunction is a stochastic variable. Equation 8 shows that the density operator is a mixture of such wavefunctions. It is therefore tempting to regard the stochastic wavefunction as providing a description of the evolution of a single quantum state, the stochastic process being provided by the environment (which includes the process of observation). Percival and his co-workers particularly stress this viewpoint; the problem now is to relate the stochastic process to fundamental physics. The problem, as we shall see, is that there is considerable freedom in choosing the unravellings, and this makes it difficult to make fundamental statements about them.

3 Unravellings

I shall discuss two techniques for unravelling the wavefunction and make some comments on them. The first has been extensively described by Mølmer; the second is Percival's quantum state diffusion. We always assume that equation 4 is known, so that we know all the \hat{L}_j Lindblad operators. The stochastic wavefunction must remain normalized, and when used in equation 8 must give $\hat{\rho}$, the solution of the master equation 4.

3.1 The Monte Carlo wavefunction

This unravelling has been widely used in quantum optics. The prescription, which mirrors the physical process of $e g$ decay, is

1. Construct the non-Hermitian Hamiltonian

$$\hat{H}_{\text{eff}} = \hat{H} - \frac{i}{2} \sum_j \hat{L}_j^\dagger \hat{L}_j \quad (9)$$

and use this to propagate the wavefunction for time dt , to get $|\Psi^1(t + dt)\rangle$ where

$$|\Psi^1(t + dt)\rangle = (1 - i\hat{H}_{\text{eff}}) |\Psi(t)\rangle \quad (10)$$

Because \hat{H}_{eff} is not Hermitian $|\Psi(t + dt)\rangle$ is not normalized. In fact, we have

$$\langle \Psi^1(t + dt) | \Psi^1(t + dt) \rangle = 1 - dp \quad (11)$$

with

$$dp = \sum_j dp_j \quad (12)$$

and

$$dp_j = dt \langle \Psi(t) | \hat{L}_j^\dagger \hat{L}_j | \Psi(t) \rangle (\geq 0) \quad (13)$$

The value of dt must be chosen so that $dp \ll 1$

2. We now introduce the stochastic development. Choose a random number ϵ , between 0 and 1 and compare with dp
3. If $dp < \epsilon$ (as it usually is) then no jump occurs and we simply normalize the wavefunction, so that

$$|\Psi(t + dt)\rangle = \frac{|\Psi^1(t + dt)\rangle}{\sqrt{(1 - dp)}} \quad (14)$$

but

4. If (unusually) $dp > \epsilon$ a 'quantum jump' occurs and we take, with probability

$$\begin{aligned} \Pi_j &= dp_j / dp \\ |\Psi(t + dt)\rangle &= \frac{\hat{L}_j |\Psi(t)\rangle}{\sqrt{dp_j / dt}} \end{aligned} \quad (15)$$

We have to show that this is equivalent to the master equation. At time $t + dt$ the density operator is

$$\hat{\rho}(t + dt) = \langle \overline{|\Psi(t + dt)\rangle\langle\Psi(t + dt)|} \rangle$$

where the overbar represents the average over all the probabilistic evolutions of the wavefunction $|\Psi(t)\rangle$ from t to $t + dt$ and the average $\langle \dots \rangle$ is the average over all stochastic realizations of $|\Psi(t)\rangle$ at time t . Considering the probabilistic evolution described above first, we have

$$\overline{|\Psi(t + dt)\rangle\langle\Psi(t + dt)|} = (1 - dp) \frac{|\Psi^1(t + dt)\rangle\langle\Psi^1(t + dt)|}{\sqrt{(1 - dp)}} + \sum_j dp_j \frac{\hat{L}_j |\Psi(t)\rangle\langle\Psi(t)| \hat{L}_j^\dagger}{\sqrt{dp_j/dt} \sqrt{dp_j/dt}} \quad (16)$$

Now we use equations 9 and 10 in equation 16 to get

$$\begin{aligned} \overline{|\Psi(t + dt)\rangle\langle\Psi(t + dt)|} &= |\Psi(t)\rangle\langle\Psi(t)| - idt[\hat{H}, |\Psi(t)\rangle\langle\Psi(t)|] \\ &\quad - dt/2 \sum_j \left(\hat{L}_j^\dagger \hat{L}_j |\Psi(t)\rangle\langle\Psi(t)| + |\Psi(t)\rangle\langle\Psi(t)| (\hat{L}_j \hat{L}_j^\dagger) \right) \\ &\quad + dt \sum_j \hat{L}_j |\Psi(t)\rangle\langle\Psi(t)| \hat{L}_j^\dagger \end{aligned} \quad (17)$$

Now doing the $\langle \dots \rangle$ average over $|\Psi(t)\rangle$ in equation 17 we reproduce equation 4.

In summary, an average over the stochastic wavefunctions generated by the Monte Carlo procedure described above is indistinguishible from the solution of the master equation.

3.2 Physical interpretation in the case of decay

Let us now consider a 2-level system which starts in the state

$$|\Psi(0)\rangle = \alpha_0|0\rangle + \beta_0|1\rangle = \begin{bmatrix} \alpha_0 \\ \beta_0 \end{bmatrix}$$

Let us take

$$\begin{aligned} \hat{H} &= \omega_0/2 \{1 - \sigma_z\} = \begin{bmatrix} 0 & 0 \\ 0 & \omega_0 \end{bmatrix} \\ \hat{L}_1 &= \sqrt{\gamma} \sigma_+ = \begin{bmatrix} 0 & \sqrt{\gamma} \\ 0 & 0 \end{bmatrix} \end{aligned}$$

which corresponds to spontaneous decay. Notice

$$\hat{L}_1^\dagger \hat{L}_1 = \gamma/2 \{1 - \sigma_z\} = \begin{bmatrix} 0 & 0 \\ 0 & \gamma \end{bmatrix}$$

is the projector onto the ground state. Now it is easy to solve for $|\Psi^1\rangle$

$$|\Psi^1(dt)\rangle = \begin{bmatrix} \alpha_0 \\ \beta_0 \exp(-i\omega_0 dt) \exp(-\gamma dt/2) \end{bmatrix} \quad (18)$$

whence we see that the probability of making a jump is just

$$dp = \gamma |\beta_0|^2 dt \quad (19)$$

If a jump is made, the normalized wavefunction is

$$|\Psi(dt)\rangle_{\text{jump}} = |0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

that is, in time dt the system has decayed with probability $\gamma dt \times$ (probability of being in the excited state). Something more interesting happens if no jump occurs in time dt . We calculate $|\Psi(dt)\rangle$ by normalizing $|\Psi^1(dt)\rangle$, and this gives us (to first order in dt)

$$|\Psi(dt)\rangle_{\text{nojump}} = \alpha_0 \left(1 + \frac{\gamma dt |\beta_0|^2}{2}\right) |0\rangle + \beta_0 \left(1 - \frac{\gamma dt |\alpha_0|^2}{2}\right) |1\rangle = \begin{bmatrix} \alpha_0 \left(1 + \frac{\gamma dt |\beta_0|^2}{2}\right) \\ \beta_0 \left(1 - \frac{\gamma dt |\alpha_0|^2}{2}\right) \end{bmatrix} \quad (20)$$

Thus, in this form of unravelling, if no jump occurs, the wavefunction rotates; the probability of being in the ground state increases while the excited state probability falls. We can actually solve for a finite period of length t without jumps, to get

$$|\Psi(t)\rangle = \alpha(t)|0\rangle + \beta(t)|1\rangle = \begin{bmatrix} \alpha(t) \\ \beta(t) \end{bmatrix} \quad (21)$$

with

$$\alpha(t) = \frac{\alpha_0}{\sqrt{|\alpha_0|^2 + |\beta_0|^2 \exp(-\gamma t)}}$$

$$\beta(t) = \frac{\beta_0 \exp(-\gamma t/2)}{\sqrt{|\alpha_0|^2 + |\beta_0|^2 \exp(-\gamma t)}}$$

We may interpret this as the change in wavefunction which results from our knowledge of the circumstance that it has gone for a time t without decay. The longer t , the more likely the wavefunction is in its ground state. More examples can be found in [5].

3.3 The state diffusion wavefunction

Unravellings are not unique. Percival [10] writes his quantum state diffusion equation as the Itô stochastic differential equation ($\langle \hat{L} \rangle_\psi = \langle \psi | \hat{L} | \psi \rangle$)

$$|d\psi\rangle = -i\hat{H}|\psi\rangle dt + \sum_j \left(\langle \hat{L}_j^\dagger \rangle_\psi \hat{L}_j - \frac{1}{2} \hat{L}_j^\dagger \hat{L}_j - \frac{1}{2} \langle \hat{L}_j^\dagger \rangle_\psi \langle \hat{L}_j \rangle_\psi \right) |\psi\rangle dt + \sum_j \left(\hat{L}_j - \langle \hat{L}_j \rangle_\psi \right) |\psi\rangle d\xi_j, \quad (22)$$

where the $d\xi_j$ are independent complex differential Gaussian random variables satisfying the conditions

$$M d\xi_j = M d\xi_i d\xi_j = 0, \quad M d\xi_i^* d\xi_j = \delta_{ij} dt, \quad (23)$$

where M denotes the ensemble mean. This equation is also equivalent to the master equation, as can be seen by writing

$$|\psi(t+dt)\rangle = |\psi(t)\rangle + |d\psi\rangle$$

using equation 22 for $|d\psi\rangle$ and evaluating the ensemble mean. This form of unravelling is particularly interesting if \hat{L} corresponds to an observable, (and is therefore Hermitian), so that 22 can be simplified to

$$|d\psi\rangle = -i\hat{H}|\psi\rangle dt - \frac{1}{2} \hat{L}_\Delta^2 |\psi\rangle dt + \hat{L}_\Delta |\psi\rangle d\xi \quad (24)$$

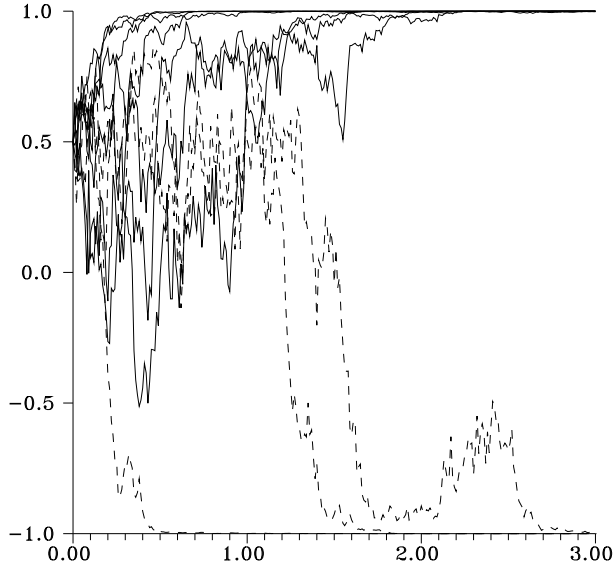


Figure 1: The value of $\langle \sigma_z \rangle$ for 10 trajectories as a function of time (arbitrary units). Three trajectories (dotted) converge to -1, seven (solid) to +1. All start in the state $\sqrt{3}/2|\uparrow\rangle + i/2|\downarrow\rangle$

with

$$\hat{L}_\Delta = \hat{L} - \langle \hat{L} \rangle_\psi$$

This implies that any fluctuation which takes $|\psi\rangle$ towards an eigenstate of \hat{L} reduces \hat{L}_Δ , so the wavefunction has smaller fluctuations. Eventually, $|\psi\rangle$ will become stuck in one of the eigenstates of \hat{L} and \hat{L}_Δ will vanish. Subsequent time development is then due to \hat{H} alone. This provides a model for quantum observation.

4 Summary

I have described two types of unravelling of the master equation into stochastic wavefunctions. Each provides insights into the way in which the environment may influence the wavefunction. Unfortunately, unravellings are not unique, and information contained in the unravellings is lost when the mean is taken to get the density operator. We therefore have to be careful about what we put into the unravellings, if we want to interpret them. They may be most useful for solving large problems, but not much work seems to have been done on this.