How to Probe for Dynamical Structure in the Collapse of Entangled States Using Nuclear Magnetic Resonance

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May 29, 1997

Abstract

The spin state of two magnetically inequivalent protons in contiguous atoms of a molecule becomes entangled by the indirect spin-spin interaction (j-coupling). The degree of entanglement oscillates at the beat frequency resulting from the splitting of a degeneracy. This beating is manifest in NMR spectroscopy as an envelope of the transverse magnetization and should be visible in the free induction decay signal. The period (≈ 1 sec) is long enough for interference between the linear dynamics and collapse of the wave-function induced by a Stern-Gerlach inhomogeneity to significantly alter the shape of that envelope. Various dynamical collapse theories can be distinguished by their observably different predictions with respect to this alteration. Adverse effects of detuning due to the Stern-Gerlach inhomogeneity can be reduced to an acceptable level by having a sufficiently thin sample or a strong rf field.

Pacs:03.65.Bz - quant-ph 9706002

The measurement problem of quantum mechanics arises because the theory is silent as to when and how the transition takes place in dynamical processes between linear, deterministic Schrödinger evolution, and non-linear, stochastic wave-function collapse. One can sweep this problem under the rug only so long as experimental probes are unable to enter the transition region. Advancing techniques in mesoscopic physics make such an entry possible. The purpose of this paper is to suggest that we may already be able to investigate the transition region using well-developed techniques of nuclear magnetic resonance (NMR).

To see how we might go about distinguishing one theory of wave function collapse from another, let us suppose that we can arrange a dynamical transformation which, during a time $t_e$, causes the following evolution of the spin state of two spin-1/2 particles:

$$|\downarrow\rangle|\downarrow\rangle \rightarrow 2^{-1/2}(|\downarrow\rangle|\downarrow\rangle + |\uparrow\rangle|\uparrow\rangle) \rightarrow |\downarrow\rangle|\downarrow\rangle.$$  

(1)

Suppose further that during this evolution an inhomogeneous (Stern-Gerlach) magnetic field is used as a measuring device, the result of the measurement being that the system collapses into one of the states $|\downarrow\rangle|\downarrow\rangle$ or $|\uparrow\rangle|\uparrow\rangle$. Spatial separation produced by a Stern-Gerlach field is proportional to the square of the time, and the spreading of the initially localized wave function is linear in the time, so there is a time $t_{sg}$ at which the ratio becomes unity, and we have a resolution of the two states.

Consider now what will happen if we arrange to have:

$$t_e \approx t_{sg}.$$  

(2)

Two types of entanglement occur: the spin-spin entanglement occurring in (1) and the entanglement of spin and space parts of the wave function as the latter separates into non-overlapping fragments under the influence of the Stern-Gerlach field. One type of theory of wave-function collapse known as “spontaneous localization theory” (SLT)$^{3,4}$ attributes all collapse to spatial separation. In such theories the entangled state $2^{-1/2}(|\downarrow\rangle|\downarrow\rangle + |\uparrow\rangle|\uparrow\rangle)$ is not driven to collapse until the spatial separation has taken place. The situation is quite different, however, in another type of theory known as “induced non-linearity theory” (INL). In such theories any linear hamiltonian which is able to distinguish the factorized constituents of an
entangled state must induce a non-linear term that brings about collapse. If INL theory were correct, the presence of the inhomogenous magnetic field would induce a non-linear term that would push the entangled spin-spin state towards collapse as that state is forming. Competition with the linear hamiltonian would thus occur all during the interval $0 < t < t_{sg}$. Stopping process (1) at various times $t$ in this interval leaves the system in different states for the two theories, and this difference can have observable consequences.

We are now going to show that this scheme for testing a collapse theory experimentally can be implemented using two proton spins in contiguous atoms $A$ and $A'$ of a molecule $AA'$.

To begin with we must distinguish the sort of measurement we have in mind from conventional NMR spectroscopy. NMR spectroscopy probes the internal dynamics by detecting shifts in the Larmor frequency $\omega$ in a strong static magnetic field $B$. If one applies a transverse magnetic field of magnitude $b << B$ in a narrow frequency band including $\omega$, the dynamical effect is as if one moved to a frame rotating with the Larmor frequency. In this frame the static field appears much weaker, and the transverse field appears to be static. The internal dynamics then competes with the weakened magnetic interaction, and the eigenfrequencies of the resulting hamiltonian carry information about the dynamics. Since these frequencies also control the fourier distribution of the transverse magnetization, they can be detected by turning off the transverse field and fourier analyzing the free induction decay signal which appears as the spins relax. It is essential to maintain a high degree of homogeneity of the static field to prevent detuning of the Larmor frequency. But the testing of collapse dynamics requires that the field be inhomogeneous, and hence we cannot simply make use of small frequency shifts as a probe.

To obtain such a probe we must find an experimental manifestation of entanglement that is relatively insensitive to detuning. Fortunately, as we shall see, such a manifestation will be found in a remarkable correlation between the degree of entanglement and a low frequency envelope of the transverse magnetization (ETM). This correlation appears because both the entanglement and the ETM are produced by the same mechanism: a beating between two frequencies split by spin-spin interaction:

The dynamical situation of the two protons that we are going to exploit is the following: A difference in their electronic environments produces a different “chemical shift” of their magneto-gyric ratios and thereby of their Larmor frequencies. This effect is proportional to the B field strength and typically $\sim 10$ppm (parts per million). There is a still smaller but measurable effect of the indirect spin-spin interaction (j-coupling) which is transmitted from one spin to the other via a distortion in the electronic wave function. The j-coupling, being a two-particle interaction, will entangle a spin-spin state provided that the state is not one of its eigenstates. Because of the chemical-shift the coupling to an external magnetic field is not simply proportional to a component of the angular momentum, and hence it does not commute with the j-coupling. Thus the state is not an eigenstate of the j-coupling and will become entangled. The frequency shift due to j-coupling is of order $j \approx 1Hz$ (it is independent of the external field) and so the entanglement time $t_e$ will be of the order of seconds.

Let us compare this with the Stern-Gerlach separation time $t_{sg}$. For $dB/dz \approx 1T/cm$ we have

$$t_{sg}^{-1} = \frac{\gamma D}{\hbar} \frac{dB}{dz}.$$  

(3)

where $\gamma$ is the average magneto-gyric ratio for the two protons and $D$ is the molecular diameter. One finds that this is also of the order of seconds, so we have the required condition $t_{sg} \approx t_e$.

Our next step is to examine the relationship between the entanglement and the transverse magnetization

$$M = (\langle \psi | \sigma_x / 2 | \psi \rangle)^2 + (\langle \psi | \sigma_y / 2 | \psi \rangle)^2)^{1/2}. $$

(4)

As shown in reference (5) there is a natural measure of entanglement:

$$E(\psi) \equiv 2 | \det C | = 2 | C_{11} C_{22} - C_{12} C_{21} |. $$

(5)

for the general state:

$$| \psi(t) \rangle = C_{11} (t) | \uparrow \rangle | \uparrow \rangle + C_{22} | \downarrow \rangle | \downarrow \rangle + C_{12} (t) | \uparrow \rangle | \downarrow \rangle + C_{21} (t) | \downarrow \rangle | \uparrow \rangle. $$

(6)
One verifies that $E$ ranges from 0 for factorized states to 1 for maximally entangled states. To compute $E$ and $M$ we must next determine the evolution of the state $|\psi(t)\rangle$ with and without the INL contribution.

The Hamiltonian describing two protons with magneto-gyric ratios $\gamma_1, \gamma_2$ in a magnetic field $B$ is

$$H_B = \left(\frac{\gamma_1}{2} \sigma^{(1)} + \frac{\gamma_2}{2} \sigma^{(2)}\right) \cdot B = \frac{1}{4} \left((\gamma_1 + \gamma_2) \sigma + (\gamma_1 - \gamma_2) \delta \sigma\right) \cdot B,$$

$$\sigma \equiv \sigma^{(1)} + \sigma^{(2)}, \quad \delta \sigma \equiv \sigma^{(1)} - \sigma^{(2)}.$$

The term with $\gamma_1 - \gamma_2$ in $H_B$ is the chemical shift. We take the static contribution to be of magnitude $b$ in the $z$-direction and the rf contribution to be of magnitude $\nu$, rotating in the $x$-$y$ plane with frequency $\omega$. The $j$-coupling Hamiltonian will be taken to be:

$$H_j = j\sigma^{(1)} \cdot \sigma^{(2)}.$$  

Going to a frame rotating with the frequency $\omega$ of the rf field, we obtain the effective spin part of the Hamiltonian:

$$H' = \frac{1}{2} \{\nu \sigma_z + d \delta \sigma_z + 2j \sigma^1 \cdot \sigma^2 + \lambda \sigma_z\},$$

$$\nu = \bar{\omega} - \omega, \quad d = \frac{1}{2}(\omega_1 - \omega_2), \quad \lambda = (b/B)\bar{\omega}.$$

$$\omega_1 = \gamma_1 B, \quad \omega_2 = \gamma_2 B, \quad \bar{\omega} = \frac{1}{2}(\omega_1 + \omega_2).$$

Here we have assumed that $b << B$ and so omitted the contribution of the chemical shift to the rf term. The parameter $\nu$, called the “detuning”, indicates the difference between the mean Larmor frequency of the two protons and that of the rf oscillation. Since we keep $\omega$ fixed, the variation in $\nu$ comes from the difference in the value of $\bar{\omega}$ for molecules in different parts of the sample due to the inhomogeneity of the Stern-Gerlach field.

The matrix

$$H' = \begin{pmatrix} j - \nu & 0 & \lambda/2 & \lambda/2 \\ 0 & j + \nu & \lambda/2 & \lambda/2 \\ \lambda/2 & \lambda/2 & -j + d & 2j \\ \lambda/2 & \lambda/2 & 2j & -j - d \end{pmatrix}$$

represents $H'$ in the basis:

$$|1\rangle = |\uparrow\rangle|\uparrow\rangle, \quad |2\rangle = |\downarrow\rangle|\downarrow\rangle, \quad |3\rangle = |\uparrow\rangle|\downarrow\rangle, \quad |4\rangle = |\downarrow\rangle|\uparrow\rangle.$$  

The period of $E$ can be deduced quite simply: For $j = 0$ the odd terms in the characteristic polynomial for $H'$ vanish, and so the eigenvalues have the form $\pm\kappa_0, \pm\kappa_1$ with $0 < \kappa_0 < \kappa_1$. With $j > 0$ these are perturbed, and in the parameter range above we find to first approximation:

$$\pm\kappa_0 \rightarrow \pm\kappa_0 + j, \quad \pm\kappa_1 \rightarrow \pm\kappa_1 - j.$$  

Now observe that when we compute $E$ we will encounter sums of products of two exponentials of the form $e^{i\omega t}$ and $e^{i\omega' t}$ where $\kappa, \kappa'$ are any of the four eigenvalues given in (12). One sees that there is only one low frequency that can be obtained from a combination $\kappa + \kappa'$, namely $\pm 2j$. In fact one obtains to lowest order in $j$:

$$E = (1 + \nu^2/\lambda^2)^{-1} |\sin(2jt)| \rightarrow t_e = \pi/(2j).$$

provided that $j << \nu$. Thus one sees that the entanglement results from beating between the pair $|\kappa_0 \pm j|$ or between the pair $|\kappa_1 \pm j|$. If the initial state is $|j\rangle|\downarrow\rangle$ one finds that the dominant contribution comes from the former.
These observations provide an important piece of information about the range of the detuning parameter \( \nu \) in which we shall be interested. Because \( \kappa_0 \to 0 \) if \( \nu \to 0 \) the beating is greatly reduced for zero detuning. But the factor \((1 + \nu^2/\lambda^2)^{-1}\) in (13) also reduces the entanglement as \( \nu \) becomes comparable to \( \lambda \), and so there is a middle range between \( j \) and \( \lambda \) in which the entanglement is significant.

We next perform a numerical computation to examine the relationship between \( M \) and \( E \) for a choice of parameters that are expected to produce observable correlation. For protons at \( B = 1T \) (\( \bar{\omega} \approx 40 \text{ MHz} \)) a chemical shift of 10 ppm corresponds to \( s = 400 \text{ Hz} \). It is convenient to choose our energy or time unit such that \( d = 1 \). We choose an rf field with \( b = 1G \) which gives \( \lambda = 10 \) in our units, and we choose \( j = 1Hz \) which is 0.0025 in our units. We choose \( \nu = 5 \) as typical for the range \( 1 \leq \nu \leq \lambda \).

In Figure 1 the transverse magnetization \( M \) is plotted in the absence of \( j \)-coupling so that there is no entanglement. In Figure 2 with \( \nu = 0.0025 \) the disentanglement \((1 - E)\) falls from unity to a minimum and then rises back to unity in approximately 1.5 sec, and the envelope of the transverse magnetization is visibly correlated with it.

We next determine how the envelope is altered if, as the INL theory asserts, there is competition between the collapse mechanism and the linear dynamics during the interval \( 0 < t < t_e \) when \( t_e \approx t_{sg} \). To do so we must first apply the INL theory of reference (5) to deduce the non-linear term appropriate to the experiment under consideration: The strength \( \eta \) of the term is determined by the reciprocal of the time \( t_{sg} \) required for the measuring device to recognize the factorized constituents of the spin-spin entangled state. Having arranged that \( t_{sg} \approx t_e \), it follows from (13) that we must choose \( \eta \approx 2 \). Since the Stern-Gerlach effect acts primarily on the states \(| \uparrow \rangle | \uparrow \rangle, | \downarrow \rangle | \downarrow \rangle \) we may let the non-linear term act only in the subspace of the four dimensional spin space spanned by these two states. The stochastic element of the theory is introduced by a random fluctuation in the sign of the non-linear term. This also occurs in times \( \sim t_{sg} \) and, since the proposed experiment is confined to \( 0 < t < t_{sg} \), we may ignore this fluctuation.

The non-linear, stochastic Schrödinger equation of reference (5) as applied to the experiment under consideration can now be reduced to:

\[
\frac{d}{dt} \begin{pmatrix} C_{11} \\ C_{22} \\ C_{12} \\ C_{21} \end{pmatrix} = -i \begin{pmatrix} j - \nu & 0 & \lambda/2 & \lambda/2 \\ 0 & j + \nu & \lambda/2 & \lambda/2 \\ \lambda/2 & \lambda/2 & -j + 1 & 2j \\ \lambda/2 & \lambda/2 & 2j & -j - 1 \end{pmatrix} \begin{pmatrix} C_{11} \\ C_{22} \\ C_{12} \\ C_{21} \end{pmatrix} + \eta e^{i \arg \det C} \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} C_{11}^* \\ C_{22}^* \\ C_{12}^* \\ C_{21}^* \end{pmatrix}.
\]

The factor \( e^{i \arg \det C} \) becomes indeterminate for \( \det C \to 0 \), i.e. when the state factorizes. At this point the non-linear term turns off, which means that we may evaluate the expression as zero when it becomes indeterminate. The complex conjugation operation in the last term is an essential feature of the INL theory, the significance of which will be discussed below.

The task of integrating (15) is greatly simplified in our parameter range by the observation that \( \arg \det C \) is very nearly a constant during \( 0 < t < t_{sg} \). The reason is the following: Suppose first that \( \eta = 0 \). If we compute \( C \) in the basis where \( H' \) is diagonal, we find that \( \arg \det C = \pi/2 \) at all times. Since \( j \) is small, the transformation to that basis can be approximated by a tensor product of two one-particle transformations, and such transformations leave \( \det C \) invariant. Thus for \( \eta = 0 \) we conclude that \( \arg \det C \) remains close to \( \pi/2 \) for \( 0 < t < t_e \). Since \( \eta \approx 2j \ll 1 \) in our computations, we expect that this conclusion remains valid when the non-linear term is present. Suppose tentatively that this is the case. Then the four equations (15) together with the four complex conjugate equations are a linear system of eight equations which can be readily solved. We can then check the validity of our approximation by self-consistency, i.e. computation of \( \arg \det C \) from the linearized solution and verification that it is indeed approximately \( \pi/2 \).

Figure 3 gives \( \arg \det C \) for \( \eta = 0 \) (the near step function), the other curve being a plot of \( \arg \det C \) calculated in the linearized theory for \( \eta = 2j \). Evidently the approximation is self-consistent in the first half of the interval, though deviations from the predictions of the linearized equation may be expected in the second half.
Figure 4 shows the transverse magnetization for $\eta = 2j$ as calculated from the linearized equation. Its salient feature is a strong depression of the envelope as time approaches midpassage. This feature is not an artifact of the linear approximation because, as we have shown, that approximation is accurate during the first half of the period.

Thus we arrive at a principal result of this paper: \textit{INL theory predicts a descent of the envelope of the transverse magnetization at times approaching the middle of the entanglement period.}

This descent will be found so long as the detuning is in the range $1 \lesssim \nu \lesssim \lambda$. If we assume that the gradient of the Stern-Gerlach field is $dB/dz = 1$ T/cm, we will have such a range over 90\% of the sample if the thickness is 1 micron. This restriction can be relieved by raising the strength of the rf field. Thus if $b = 10$G the sample size can be increased to 10 microns with a corresponding increase in the effective signal. Ideally an experiment should first verify the presence of an envelope in the transverse magnetization that has the form of Figure 2 in a homogeneous B field, and then ascertain whether or not it deforms to that of Figure 4 when $dB/dz$ is of the order 1T/cm. The size of the deformation will place a bound on $\eta$, with $\eta \ll 2j$ indicating failure of the INL theory. The absence of any change from Figure 2 when B is made inhomogenous would be consistent with spontaneous localization or with the commonly held view that collapse takes place instantaneously when one of the two factorized constituents is detected.

To conclude we shall comment on the physics underlying the envelope distortion produced by the INL collapse mechanism: It was shown in reference 5 that the INL theory predicts a small CP violation in the decay of neutral K mesons which, with a very coarse model, comes within 20\% of the experimental value. Neutral kaons are entangled states of $\bar{d}s$ and $s\bar{d}$ quarks, and the non-linear term is induced by the semi-leptonic decay modes which can distinguish the factorized constituents. The source of the CP symmetry-breaking is the complex conjugation operation in the INL theory. Let us now show that the strong distortion of the transverse magnetization seen in Figure 4 is also a consequence of the complex conjugation operation in (15):

Let the matrix appearing in the non-linear term be denoted $\Upsilon$. It is anti-symmetric and has non-vanishing elements only in the (12) and (21) position. When we transform to the eigenbasis of $\mathcal{H}'$ it will be seen that $\Upsilon \rightarrow \Upsilon'$ in which the latter is still anti-symmetric and has small off-diagonal elements except in the positions (12) and (21). In this basis the linear term produces oscillations $e^{-i\alpha t}$ with $\alpha$ one of the four eigenvalues $\kappa_0 - j, -\kappa_0 - j, \kappa_1 + j$, and $-\kappa_1 + j$. Because of the form of $\Upsilon'$ just noted, the non-linear term produces a large coupling between the first two only. Were it not for the complex conjugation in the non-linear term, this would have little effect because of the large frequency mismatch $(2\kappa_0)$ between $\kappa_0 - j$ and $-\kappa_0 - j$. But, because of the complex conjugation, the coupling is between $\kappa_0 - j$ and $-(\kappa_0 - j)$ so that the mismatch is only $2j$. We thus have a near resonance between the linear and non-linear term and so obtain a large effect from a small perturbation that persists over the long entanglement period.

The origin of the complex conjugation operation is the time-reversal operator, the occurrence of which in the INL theory expresses the fact that while there is no arrow of time in microscopic processes, that symmetry is broken whenever a measurement is registered. Thus, if the INL theory is correct, it is this most basic attribute of the measurement process that manifests itself both in the CP asymmetry described in reference (5) and in the ETM depression described in this paper.

\textit{Acknowledgments:} The author thanks S. Bhagat and A. Dragt for helpful discussions.

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Figure Captions

Figure 1: Transverse magnetization for no entanglement \((j = 0)\) and a homogeneous \(B\) field.

Figure 2: Correlation between transverse magnetization and entanglement \((j = .0025)\). \(B\)-field homogeneous.

Figure 3: Arg Det \(C\) for \(\eta = 0\) (the near step function) and for \(\eta = 2j\).

Figure 4: Transverse magnetization when there is entanglement \((j = .0025)\) and INL collapse \((\eta = 2j)\).
Figure 1
Figure 2
Figure 3
Figure 4