**Abstract**

In this paper we propose that anomalous Compton neutron scattering data indicative of a partial loss of scattering targets in many molecules, polymers and metallic hydrides can be explained by the existence of low-lying entangled states in the protonic or deuteronic vibrational spectrum. This entanglement is shown to be a direct result of dipolor interactions, that may be either between close neighbours or else mediated at distance by a shared coherent electric field, as described by the Tavis-Cummings model.

# 1 Introduction

Neutron Compton scattering from many hydrogenic materials yields anomalously low cross-sections indicative of a partial loss of scattering centres [1]. Materials that have been found to exhibit this effect include $H_2O$, $D_2O$, together with many polymers and transition metal hydrides [2]. We share the generally accepted view that this apparent partial disappearance of the scattering targets (protons and deuterons) must be due to some form of quantum entanglement of nucleii in the target. It has been observed that the anomaly invariably increases with neutron scattering angle ($\Theta$) and disappears as $\Theta \rightarrow 0$. Transferred momentum increases with $\Theta$ and the scattering interaction time ($\tau$) is inversely proportional to transferred momentum [3]. It has therefore been argued [1] that the entanglement responsible for the apparent loss of scattering centres is characterized by very short decoherence times on the order 1 femtosecond.

In this short paper we will disclose an alternative interpretation of the anomalous data in which decoherence time does not play a direct role in the putative mechanism.

# 2 Dipolar entanglement

When we speak of the vibration modes of a molecule involving the motion of a light nucleus (e.g. H or D) bound to a much heavier one, it is often overlooked that these are entirely quantum in nature. In the Born-Oppenheimer approximation (BOA) the light nucleus sits in a stationary effective 1-particle potential well, the 1-particle Schrödinger eigenstates of which form a spectrum with levels separated by the vibrational frequencies. The so-called vibration is more properly to be understood as a time-dependent superposition of the ground state and some excited state in the single-particle Hilbert space. The apparent vibrational oscillation is an artefact of the way in which the probability distribution moves with the relative phases of the two eigenstates. The amplitude of the vibration is hence quantised and comparable to the spatial extent of the wavefunctions $\psi_i$ of a *nucleus*. This spatial extent is many orders of magnitude greater than what we normally regard as the (femtometric) size of a nucleus.

The lowest excited states are generally of odd parity along a point symmetry axis. Hence each vibration mode of a hydrogen nucleus is associated with a electric dipole transition moment, $\mu = e < \psi_0^\dagger|\mathbf{r}|\psi_j >$. Now where there are charged dipoles there are electromagnetic couplings. These are of two kinds: longitudinal Coulomb dipole-dipole interactions that scale as $\frac{\mu^2}{R^3}$ and photon-mediated transerse couplings to the real $\mathbf{E}(\mathbf{r}, t)$ field. Both of these types of interaction are collective in the sense that they increase with particle number, but the longitudinal interactions are intrinsically short-range compared to the transverse ones that potentially involve a large number of particles coupled to a single photon mode. An $H_2O$ molecule would constitute a system of the first type, whereas a transition metal hydride such as PdH would exemplify the second type.

The odd-parity excitation energy depends upon the curvature of the effective H (D) potential but is on the order of 0.1eV in all the systems in which the anomaly has been observed. The corresponding dipole is typically on the order of 0.1e Å.

## 2.1 Diatomic dipole-dipole interaction

In molecules with two H or D nuclei with equilibrium separation $|\mathbf{r}_1 - \mathbf{r}_2|$, the otherwise degenerate first excited states will be split by a longitudinal dipole-dipole interaction $\pm\frac{\mu^2}{4\pi\epsilon_0|\mathbf{r}_1-\mathbf{r}_2|}$. Transverse geometries are also possible, but the 1D-longitudinal case suffices to illustrate the general point. The four lowest energies $E_i$ and pair states of a molecule centred at the origin are going to be of the general form:

| $E$ | $\psi(\mathbf{r}_1,\mathbf{r}_2)$ |
|---|---|
| $2E_0$ | $\psi_0(\mathbf{r}_1)\psi_0(\mathbf{r}_2)$ |
| $E_0+E_1-\frac{\mu^2}{4\pi\epsilon_0\lvert\mathbf{r}_1-\mathbf{r}_2\rvert}$ | $\psi_0(\mathbf{r}_1)\psi_1(\mathbf{r}_2)-\psi_1(\mathbf{r}_1)\psi_0(\mathbf{r}_2)$ |
| $E_0+E_1+\frac{\mu^2}{4\pi\epsilon_0\lvert\mathbf{r}_1-\mathbf{r}_2\rvert}$ | $\psi_0(\mathbf{r}_1)\psi_1(\mathbf{r}_2)+\psi_1(\mathbf{r}_1)\psi_0(\mathbf{r}_2)$ |
| $2E_1$ | $\psi_1(\mathbf{r}_1)\psi_1(\mathbf{r}_2)$ |

We need look no further for the existence of entangled states than this simple table.
The neutron scattering can only promote a target proton from its vibrational ground state into these entangled states if its own loss of energy:

$$\Delta E = E\sin^2\Theta$$

... exceeds the dipole transition energy $E_1 - E_0$
The kinetic energy $E$ of the incident neutron beam is is typically on the order of 1eV, which is consistent with the observation that the anomalous loss in effective cross-section disappears at small scattering angles.

## 3 Cooperative transverse field-dipole coupling

Following [4] we will take the basic Tavis-Cummings Hamiltonian for systems comprising many two-state hydrogen nucleii sharing a coherent quantized electric field as being:

$$H_0 = \hbar\omega a^\dagger a + \hbar\omega\left[\frac{N_s}{2} + S_3\right] + g(a^\dagger S_+ + aS_-) \tag{1}$$

...where $\hbar\omega = |E_i - E_j|$ The validity of this simple model is contingent upon the validity of a number of simplifying assumptions:

i) The interaction between radiation field and the nucleii is sufficiently weak that the rotating wave approximation (RWA) holds. This means that the total number excitations commutes with the Hamiltonian.

ii) There is 100 percent occupancy of the available sites.

iii) We need consider only two participating states: the ground state at $E_0$ and one excited state at $E_j$ and so $\hbar\omega = E_j - E_0$. This does not necessarily means that the protons are actually two-state systems, which is very unlikely to be the case.

iv) The lifetime of the states is much longer than $\omega^{-1}$

v) The coupling of each dipole to the photon field is translationally invariant.

The field amplitude $E_0$ corresponding to a single photon in the interaction volume is given by

$$\hbar\omega = 2n^2\epsilon_0 E_0^2 N_s\Omega$$

where $n$ is the real part of the refractive index at $\omega$.
The single photon coupling $g_{ij}$ of a given two state dipole transition at one of the $N_s$ sites is accordingly given by

$$g_{ij}^2 = \frac{e^2E_0^2|<i|x|j>|^2}{(\hbar\omega)^2} = \frac{e^2|<i|x|j>|^2}{2N_s\Omega n^2\epsilon_0(\hbar\omega)^2} \approx \frac{|<i|x|j>|^2}{N_s\Omega n^2(\hbar\omega)^2} \times 9.0\times10^{-9} eVm$$

## 4 Palladium hydride

Pd is one of several transition metals that can reversibly absorb hydrogen up to the point of stoichiometry, in which every available interstitial site of octahedral (O) symmetry - is occupied by a hydrogen nucleus. As pointed out in the foregoing introduction, the large mass ratio between the H atom and the host atoms, means that the H quantum oscillation is decoupled from the motion of host atoms and the interstitial hydrogen nucleus experiences an effective static potential, with local mimina at the octahedral and tetragonal symmetry points. Furthermore, each proton is screened by the Fermi gas such that intersite p-p interactions are small. The screened protons are effectively almost neutral particles, resulting in high mobility within the lattice and a very shallow effective potential. As a consequence, even the ground state has a substantial spatial extent on the order of 0.25Å.

A single hydrogen nucleus in such an environment exhibits a spectrum of singlet, doublet and triplet state representations of the local point symmetry group. The ground state is a singlet with even parity about the minimum potential along each of the symmetry axes. The next level is, in an fcc lattice, a triplet of states with odd parity along one of the symmetry axes and an excitation energy of the order of 0.06 eV (15 THz). The real and imaginary parts of the refractive index are comparable in this part of the spectrum, so there is effectively only one internally reflected mode along each of the x,y and z axes. and a single photon is effectively normalized to a slab volume $A\lambda/2$. We conclude that nanoclusters of non-stoichiometric PdD (and PdH) are amenable to the Tavis-Cummings model in which a single photon mode is coupled to $N_s$ identical two-level quasi-atoms.
In PdH, $\Omega \approx 1.6 \times 10^{-29} m^3$, so

$$\frac{e^2}{\epsilon_0 \Omega} \approx 1.1 \times 10^{21} eVm^{-2}$$

and the dipole transition coupling coefficient is given by:

$$g_{ij}^2 \approx \frac{|<i|x|j>|^2}{N_s n^2 \hbar\omega_{ij}} \times 5.5 \times 10^{20}\ eVm^{-2}$$

We chose the $x$ axis as our dipole and E-field direction, but exactly the same results would be obtained for $y$ and $z$ axes by virtue of the fcc point symmetry at the octahedral site. $\mu_x$ dipoles can only be formed by products of states that have opposite x-parity and equal y and z parities. None of the products involving $[.+-]$,$[.-+]$,$[.--]$ formed $x$-dipoles any larger than the $[.++]$ parity states and they lie at higher energies, so we do not need to consider them. We solved the $[.++]$ proton (and deuteron) states on a 3-dimensional grid of pitch $0.25\AA$ using the semi-empirical effective potential published in [5] and were able to substantially confirm the findings of that paper. The energy levels $\epsilon_i$ (relative to the potential minimum at the octahedral symmetry point) of the ten lowest states in each of the [+++] and [-++] subgroups are listed below (in units of meV):

| i,j | $E_{i_{[+++]}}$ | $E_{j_{[-++]}}$ |
|---|---|---|
| 0 | 74 | 138 |
| 1 | 215 | 252 |
| 2 | 252 | 267 |
| 3 | 332 | 333 |
| 4 | 233 | 284 |
| 5 | 377 | 368 |
| 6 | 233 | 374 |
| 7 | 362 | 378 |
| 8 | 362 | 368 |
| 9 | 368 | 432 |

[+++] states {4,6} and {7,8} are degenerate doublets, as are the [-++] states {5,8}.
We then calculated the $x$ dipole elements. The largest ones are tabulated below, together with the photon mode coupling constants $g_{ij}\sqrt{N_s}$:

| $i_{[+++]}$ | $j_{[+--]}$ | $\lvert E_i - E_j \rvert$ | $E_{LO}$ | $\langle i \rvert x \lvert j \rangle$ | $g_{ij}\sqrt{N_s}$ |
|---|---|---|---|---|---|
| 0 | 0 | 63 | 74 | 0.18 | 0.12 |
| 1 | 0 | 78 | -138 | 0.13 | 0.10 |
| 1 | 2 | 52 | 215 | 0.20 | 0.11 |
| 1 | 3 | 118 | 215 | -0.10 | 0.13 |
| 2 | 5 | 116 | 252 | 0.10 | 0.12 |
| 2 | 7 | 126 | 252 | -0.06 | 0.08 |
| 2 | 13 | 209 | 252 | -0.03 | 0.07 |
| 3 | 2 | 65 | -267 | -0.20 | 0.13 |
| 3 | 6 | 43 | 332 | 0.23 | 0.12 |
| 3 | 9 | 100 | 332 | 0.08 | 0.08 |
| 3 | 10 | 103 | 332 | -0.10 | 0.10 |
| 4 | 4 | 51 | 233 | 0.19 | 0.11 |
| 5 | 1 | 125 | -252 | -0.07 | 0.09 |
| 6 | 0 | 95 | -138 | 0.16 | 0.15 |
| 6 | 3 | 100 | 233 | -0.21 | 0.21 |

We conclude that, even with 100 percent stiochiometry, which is hardly attainable in practice, the dipole coupling to a single photon mode is not strong enough to induce a spontaneous second order phase transition to a superradiant Dicke state. It is certainly strong enough to transform the single-H spectrum into bands of entangled states whose width is on the order of 0.01eV however. In the context of Compton neutron scattering, a neutron energy loss $\Delta E \geq 0.06$eV is expected to be associated with anomalous reduction in scattering intensity, as in the case of $H_2O$ discussed above.

## 5 Conclusions

The neutron scattering anomalies observed in a wide variety of materials may admit of a simple generic explanation predicated upon the existence of dipole transitions that give rise to inter-protonic entanglement of low-lying excited states. The interaction can be of two types, either proximal dipole-dipole or else mediated between widely separated nucleii immersed in a shared coherent electric field.

## References

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