CALCULATIONS OF NUCLEAR SPIN OPTICAL ROTATION

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Faraday rotation

PHILOSOPHICAL TRANSACTIONS.

I. Experimental Researches in Electricity.—Nineteenth Series.

Received November 6,—Read November 20, 1845.

§ 26. On the magnetisation of light and the illumination of magnetic lines of force*.
¶ i. Action of magnets on light. ¶ ii. Action of electric currents on light.
¶ iii. General considerations.

¶ i. Action of magnets on light.
2146. I HAVE long held an opinion, almost amounting to conviction, in common I

M. Faraday, Philos. Trans. R. Soc. London 136, 1 (1846)
M. Faraday, Philos. Mag. 28, 294 (1846)

β = V Bd

(Figure source: Wikipedia)
Optical detection of liquid-state NMR

I. M. Savukov¹, S.-K. Lee¹ & M. V. Romalis¹

Nuclear magnetic resonance (NMR) in liquids and solids is primarily detected by recording the net dipolar magnetic field outside the spin-polarized sample. But the recorded bulk magnetic field itself provides only limited spatial or structural information about the sample. Most NMR applications rely therefore on more elaborate techniques such as magnetic field gradient encoding¹ or spin correlation spectroscopy², which enable spatially resolved imaging and molecular structure analysis, respectively. Here we demonstrate a fundamentally different and intrinsically information-richer modality of detecting NMR, based on the rotation of the polarization of a laser beam by the nuclear spins in a liquid sample. Optical NMR detection has in fact a long history in atomic vapours with narrow resonance lines³,⁴, but has so far only been applied to highly specialized condensed matter systems such as quantum dots⁵. It has been predicted⁶ that laser illumination can shift NMR frequencies and thus aid detection, but the effect is very small and has never been observed. In contrast, our measurements on water and liquid¹⁷²⁹Xe show that the complementary effect—the rotation of light polarization by nuclear spins—is readily measurable, and that it is enhanced dramatically in samples containing heavy nuclei. This approach to optical NMR detection should allow correlated optical and NMR spectroscopy on complex molecules, and continuous two-dimensional imaging of nuclear magnetization with spatial resolution limited only by light diffraction.
Theory of magneto-optic rotation

\[ LPL = l \cdot \text{CPL}_- + r \cdot \text{CPL}_+ \]

\[
\tilde{\theta} = \frac{\omega l}{2c} (\tilde{n}_- - \tilde{n}_+) \]

Buckingham, Philos. Trans. R. Soc. London A293, 239 (1979): for \( n \approx 1 \Rightarrow \]

\[
\tilde{n}_{\epsilon \tau} = \delta_{\epsilon \tau} + \frac{N}{2\varepsilon_0} \langle \tilde{\alpha}_{\epsilon \tau} \rangle \]

where \( \tilde{\mu}_\epsilon(t) = \sum_\tau \tilde{\alpha}_{\epsilon \tau} \tilde{E}_\tau(t) \)

For a real wave function (no orbital degeneracy):

\[
\begin{align*}
\text{Re } \tilde{\alpha} & \Leftrightarrow \text{dispersion} \\
\text{Im } \tilde{\alpha} & \Leftrightarrow \text{absorption}
\end{align*}
\]

Now: \( \tilde{n}_- = \tilde{n}_{YX} ; \quad \tilde{n}_+ = \tilde{n}_{XY} \)
In the presence of magnetic interaction the wave function becomes complex and

\[ \tilde{\alpha}_{\epsilon\tau} \to \tilde{\alpha}_{\epsilon\tau} - i \tilde{\alpha}'_{\epsilon\tau} = \alpha_{\epsilon\tau} - i \tilde{\alpha}'_{\epsilon\tau} \]

where \( \alpha_{\epsilon\tau} \) is conventional symmetric polarisability. The antisymmetric polarisability

\[ \tilde{\alpha}'_{\epsilon\tau}(B_0, I_K) = \tilde{\alpha}'_{\epsilon\tau}(0, 0) + \sum_{\nu} \tilde{\alpha}'_{\epsilon\tau,\nu}(B_0) B_{0,\nu} + \sum_{\nu} \tilde{\alpha}'_{\epsilon\tau,\nu}(I_K) I_{K,\nu} + \ldots \]

[Lu, He, Chen, He & Liu, Chem. Phys. Lett. 479, 14 (2009)] arises from terms linear in either

(1) external magnetic field \( B_0 \) \( \Rightarrow \) Faraday OR
(2) field due to polarisation of nuclear spins \( I_K \) \( \Rightarrow \) NSOR

Away from optical resonances \( \tilde{\alpha} \to \alpha \) and the measurable rotation angle

\[ \Phi = \text{Re } \tilde{\theta} = \frac{1}{2} \omega l N \mu_0 c \text{ Im } \langle \alpha'_{XY} \rangle \]
Response theory formulation of time-dependent perturbation theory:
Time-dependent expectation value corresponding to observable $A$ in a state per-
turbed by frequency-dependent perturbations $B_{\omega_1}$, $C_{\omega_2}$, $D_{\omega_3}$, . . . :

$$\langle A \rangle (t) = \langle 0 | A | 0 \rangle + \int_{-\infty}^{\infty} d\omega_1 \exp (-i \omega_1 t) \langle\langle A; B_{\omega_1}\rangle\rangle_{\omega_1}$$

$$+ \frac{1}{2} \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 \exp [-i (\omega_1 + \omega_2) t] \langle\langle A; B_{\omega_1}, C_{\omega_2}\rangle\rangle_{\omega_1,\omega_2}$$

$$+ \frac{1}{6} \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 \int_{-\infty}^{\infty} d\omega_3 \exp [-i (\omega_1 + \omega_2 + \omega_3) t] \langle\langle A; B_{\omega_1}, C_{\omega_2}, D_{\omega_3}\rangle\rangle_{\omega_1,\omega_2,\omega_3}$$

$$+ \ldots$$

in terms of

- expectation value $\langle 0 | A | 0 \rangle$
- linear response function $\langle\langle A; B_{\omega_1}\rangle\rangle_{\omega_1}$
- quadratic response function $\langle\langle A; B_{\omega_1}, C_{\omega_2}\rangle\rangle_{\omega_1,\omega_2}$
- cubic response function $\langle\langle A; B_{\omega_1}, C_{\omega_2}, D_{\omega_3}\rangle\rangle_{\omega_1,\omega_2,\omega_3}$
- . . .
In terms of response functions expressed in a molecule-fixed Cartesian frame

\[
\begin{align*}
\alpha_{\epsilon\tau}(\omega) &= -\langle\mu_\epsilon; \mu_\tau\rangle_\omega \\
\alpha'_{\epsilon\tau,\nu}(\omega) &= -\langle\mu_\epsilon; \mu_\tau, h_{\nu}^{OZ}\rangle_{\omega,0} \\
\alpha'_{\epsilon\tau,\nu}(I_K)(\omega) &= -\langle\mu_\epsilon; \mu_\tau, h_{\nu}^{PSO}\rangle_{\omega,0}
\end{align*}
\]

with the orbital Zeeman (OZ) and orbital hyperfine (PSO) interactions

\[
H_{OZ} = \sum_\nu h_{\nu}^{OZ} B_{0,\nu} \quad ; \quad h_{\nu}^{OZ} = \frac{e}{2m_e} \sum_i \ell_{iO,\nu}
\]

\[
H_{PSO} = \sum_\nu h_{\nu}^{PSO} I_{K,\nu} \quad ; \quad h_{\nu}^{PSO} = \frac{e\hbar \mu_0}{m_e 4\pi \gamma_K} \sum_i \frac{\ell_{iK,\nu}}{r_{iK}^3}
\]

For \( B_0 = B_0 \hat{Z} \) or average spin polarisation \( \langle I_K \rangle = \langle I_{K,Z} \rangle \hat{Z} \), in a medium where the molecules are tumbling isotropically (gas, liquid):

\[
\langle \alpha'_{XY} \rangle = \left\{ \begin{array}{ll}
B_0 \frac{1}{6} \sum_{\epsilon\tau\nu} \varepsilon_{\epsilon\tau\nu} \alpha'_{\epsilon\tau,\nu}(B_0) \\
\langle I_{K,Z} \rangle \frac{1}{6} \sum_{\epsilon\tau\nu} \varepsilon_{\epsilon\tau\nu} \alpha'_{\epsilon\tau,\nu}(I_K)
\end{array} \right.
\]
Faraday OR:

\[ V(\omega) = \frac{\Phi_F}{B_0 l} = -\frac{1}{2} \omega N \mu_0 c \frac{e^3}{2m_e} \frac{1}{6} \sum_{\varepsilon \tau \nu} \varepsilon_{\varepsilon \tau \nu} \text{Im} \langle \langle r_\varepsilon; r_\tau, l_{O,\nu} \rangle \rangle_{\omega,0} \]

NSOR (with \( N = [ ]N_A \)):

\[ \frac{\Phi_{\text{NSOR}}}{[ ]l} = -\frac{1}{2} \omega N_A \mu_0 c \langle I_{K,Z} \rangle \frac{e^3 \hbar \mu_0}{m_e 4\pi} \gamma_K \frac{1}{6} \sum_{\varepsilon \tau \nu} \varepsilon_{\varepsilon \tau \nu} \text{Im} \langle \langle r_\varepsilon; r_\tau, \frac{\ell_{K,\nu}}{r_K^3} \rangle \rangle_{\omega,0} \]
Connection to *NMR frequency shift* $\Delta$ *due to CPL* beam of intensity $I_0$ (*inverse* Faraday effect):

$$\Phi_{\text{NSOR}} = -h \omega N_A \langle I_{K,Z} \rangle \Delta I_0$$

First-principles predictions of $\Delta/I_0$:


$\Rightarrow$ $\Delta/I_0$ is tiny, but NSOR is measurable!


*Figure 3* | Dependence of optical rotation on laser wavelength. Shown are the optical rotation angle per unit length for 1 M concentration of fully-polarized $^{129}\text{Xe}$ spins in liquid Xe (a) and protons in water (b) as a function of laser wavelength. The error bars include combined statistical ($\pm$ 1 s.d.) and systematic uncertainties. In a, the solid line is a fit to the wavelength dependence given by equation (1) with $h \omega_k = 10$ eV. The results of a MCGSF *ab initio* calculation using complete active space ‘CAS’ and restricted active space ‘RAS-II’ of atomic orbitals are shown with dashed and dash-dotted lines, respectively. In b, the solid line is the optical rotation expected from nuclear magnetization due to the Faraday effect, assuming $B = 4\pi M$ in a long cylindrical cell, that is, $\kappa_M = 1$. 

Juha Vaara (9) QCSMF, Toulouse, September 2010
Calculations

- Quadratic response using **Dalton** at Hartree-Fock, density-functional theory and coupled-cluster levels
- Both standard NIR/VIS frequencies and around optical resonances
- **Completeness-optimised** co-1 and co-2 basis sets for efficient near basis-set-limit results
Laser-induced nuclear magnetic resonance splitting in hydrocarbons

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2NMR Research Group, Department of Physical Sciences, University of Oulu, P.O. Box 3000, Oulu FIN-90014, Finland
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\[ Y(\zeta) = \sum_{m} \langle g(\zeta) | \chi_m \rangle^2 \]

FIG. 2. (Color online) $2\Delta/I_0$ for ethene at 514.5 nm at the HF level using co and cc basis sets with different numbers of basis functions ($N_{bas}$).
Results

<table>
<thead>
<tr>
<th>$\omega$ (a.u.)</th>
<th>$\lambda$ (nm)</th>
<th>HF co-2</th>
<th>BHandHLYP co-2</th>
<th>B3LYP co-2</th>
<th>BLYP co-2</th>
<th>PBE0 co-2</th>
<th>PBE co-2</th>
<th>CC2 co-2</th>
<th>CCSD co-1</th>
<th>CCSD co-2</th>
<th>Exp.</th>
<th>DFT</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0932147</td>
<td>488.8</td>
<td>3.72</td>
<td>5.02</td>
<td>4.95</td>
<td>6.53</td>
<td>8.30</td>
<td>5.93</td>
<td>7.91</td>
<td>6.61</td>
<td>5.41</td>
<td>5.52</td>
<td>5.85 [21]</td>
</tr>
<tr>
<td>0.0885585</td>
<td>514.5</td>
<td>3.33</td>
<td>4.48</td>
<td>4.42</td>
<td>5.82</td>
<td>7.38</td>
<td>5.29</td>
<td>7.03</td>
<td>5.89</td>
<td>4.83</td>
<td>4.93</td>
<td>5.24 [21]</td>
</tr>
<tr>
<td>0.0773571</td>
<td>589.0</td>
<td>2.49</td>
<td>3.34</td>
<td>3.30</td>
<td>4.32</td>
<td>5.44</td>
<td>3.93</td>
<td>5.19</td>
<td>4.38</td>
<td>3.60</td>
<td>3.67</td>
<td>3.79 [23], 3.81 [24]</td>
</tr>
<tr>
<td>0.0656249</td>
<td>694.3</td>
<td>1.76</td>
<td>2.36</td>
<td>2.32</td>
<td>3.03</td>
<td>3.80</td>
<td>2.76</td>
<td>3.63</td>
<td>3.08</td>
<td>2.54</td>
<td>2.58</td>
<td>2.66 [21]</td>
</tr>
<tr>
<td>0.0428226</td>
<td>1064.0</td>
<td>0.73</td>
<td>0.98</td>
<td>0.96</td>
<td>1.25</td>
<td>1.55</td>
<td>1.14</td>
<td>1.49</td>
<td>1.27</td>
<td>1.05</td>
<td>1.07</td>
<td></td>
</tr>
<tr>
<td>0.0345439</td>
<td>1319.0</td>
<td>0.47</td>
<td>0.63</td>
<td>0.62</td>
<td>0.80</td>
<td>1.00</td>
<td>0.73</td>
<td>0.96</td>
<td>0.82</td>
<td>0.68</td>
<td>0.69</td>
<td></td>
</tr>
</tbody>
</table>

$^a$ The exponent range of the co-1 basis is wider than that of co-2, indicating higher quality of co-1. With experimental $\mathcal{N}$ based on mass density 998.2 kg m$^{-3}$ and $R_0$ placed at the center of mass.

$^b$ Liquid-state measurements at room temperature [21], 20 C [23], and 17 C [24].

Table 2: Verdet constant $V$ in rad/(T m) for ethanol, nitromethane, and urea using different DFT functionals and \textit{ab initio} methods with the co-1 and co-2 basis sets. $^a$

<table>
<thead>
<tr>
<th></th>
<th>Ethanol (C$_2$H$_5$OH)</th>
<th>Nitromethane (CH$_3$NO$_2$)</th>
<th>Urea ([NH$_2$)$_2$CO]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>BHHandHLYP</td>
<td>B3LYP</td>
<td>BLYP</td>
</tr>
<tr>
<td>(\omega) (a.u.)</td>
<td>(\lambda) (nm)</td>
<td>co-1 co-2 co-2</td>
<td>co-1 co-2</td>
</tr>
<tr>
<td>0.0932147</td>
<td>488.8</td>
<td>3.52 3.32 3.80</td>
<td>4.24 3.67</td>
</tr>
<tr>
<td>0.0885585</td>
<td>514.5</td>
<td>3.16 2.98 3.41</td>
<td>3.79 3.29</td>
</tr>
<tr>
<td>0.0773571</td>
<td>589.0</td>
<td>2.38 2.24 2.56</td>
<td>2.84 2.47</td>
</tr>
<tr>
<td>0.0656249</td>
<td>694.3</td>
<td>1.69 1.59 1.81</td>
<td>2.02 1.75</td>
</tr>
<tr>
<td>0.0428226</td>
<td>1064.0</td>
<td>0.71 0.66 0.76</td>
<td>0.84 0.73</td>
</tr>
<tr>
<td>0.0345439</td>
<td>1319.0</td>
<td>0.46 0.43 0.49</td>
<td>0.54 0.47</td>
</tr>
</tbody>
</table>

$^a$ The center of mass of the molecule was used as the gauge origin in all calculations. The number density \(N\) appropriate to the liquid phase was applied for ethanol (mass density 789.2 kg m$^{-3}$) and nitromethane (1137.1 kg m$^{-3}$), whereas the solid-state value was used for urea (1320 kg m$^{-3}$). Gauge origin at one of the nitrogen atoms was tested for urea, with no change in results.


NSOR results

TABLE II: Calculated $\Phi_{\text{NSOR}}/([\Gamma]_l)$ [in $10^{-6}$ rad/(M cm)] for $^1$H in liquid water using different methods and basis sets. $^a$

<table>
<thead>
<tr>
<th>$\omega$ (a.u.)</th>
<th>$\lambda$ (nm)</th>
<th>HF co-2</th>
<th>BHandHLYP co-2</th>
<th>B3LYP co-2</th>
<th>BLYP co-2</th>
<th>PBE0 co-2</th>
<th>PBE co-2</th>
<th>CC2 co-2</th>
<th>CCSD co-1 co-2</th>
<th>Exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0932147</td>
<td>488.8</td>
<td>0.30</td>
<td>0.42</td>
<td>0.41</td>
<td>0.55</td>
<td>0.74</td>
<td>0.51</td>
<td>0.71</td>
<td>0.58</td>
<td>0.48</td>
</tr>
<tr>
<td>0.0885585</td>
<td>514.5</td>
<td>0.27</td>
<td>0.37</td>
<td>0.36</td>
<td>0.49</td>
<td>0.66</td>
<td>0.45</td>
<td>0.63</td>
<td>0.52</td>
<td>0.43</td>
</tr>
<tr>
<td>0.0856454</td>
<td>532.0</td>
<td>0.25</td>
<td>0.35</td>
<td>0.33</td>
<td>0.46</td>
<td>0.61</td>
<td>0.42</td>
<td>0.59</td>
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<td>0.40</td>
<td>0.39</td>
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<tr>
<td>0.0773571</td>
<td>589.0</td>
<td>0.20</td>
<td>0.28</td>
<td>0.27</td>
<td>0.37</td>
<td>0.49</td>
<td>0.33</td>
<td>0.39</td>
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<td>0.16</td>
<td>0.21</td>
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<td>0.26</td>
<td>0.26</td>
<td>0.22</td>
<td>0.19</td>
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<td>0.18</td>
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<td>0.08</td>
<td>0.08</td>
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<td>0.14</td>
<td>0.10</td>
<td>0.13</td>
<td>0.11</td>
<td>0.10</td>
</tr>
</tbody>
</table>

$^a$ Normalized to $1 \text{ M} = 1 \text{ mol dm}^{-3}$ concentration and full polarization of spins, i.e., $\langle I_z \rangle = 1/2$ for $^1$H.

$^b$ Ref. 8. Liquid-state measurement.

Enhanced chemical distinction between non-equivalent nuclei?

- Selective magnetisation — the PSO operator
- Selective excitation of chromophores — the $\mu$ operators

$\Rightarrow$

**NSOR close to optical resonance: ethanol**
TABLE III: Calculated $\Phi_{NSOR}/(|I|)$ [in $10^{-7}$ rad/(M cm)] for $^1$H in PSB11 at the BHandHLYP/co-2 level. The numbering refers to groups of equivalent nuclei.

<table>
<thead>
<tr>
<th>$\omega$ (a.u.)</th>
<th>$\lambda$ (nm)</th>
<th>47+48</th>
<th>46</th>
<th>37...39</th>
<th>40</th>
<th>49+50</th>
<th>32...34</th>
<th>26...31</th>
<th>24+25</th>
<th>22+23</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0932147</td>
<td>488.8</td>
<td>-153.45</td>
<td>-386.83</td>
<td>693.41</td>
<td>85.18</td>
<td>-174.00</td>
<td>265.29</td>
<td>-126.55</td>
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<td>148.15</td>
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<td>514.5</td>
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<td>-73.24</td>
<td>-11.95</td>
<td>30.42</td>
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<td>25.45</td>
<td>6.94</td>
<td>-7.20</td>
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<td>589.0</td>
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<td>-11.63</td>
<td>2.72</td>
<td>10.59</td>
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<td>1.43</td>
<td>2.25</td>
<td>0.72</td>
<td>2.07</td>
<td>1.58</td>
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<td>1319.0</td>
<td>0.07</td>
<td>1.82</td>
<td>-0.05</td>
<td>0.94</td>
<td>1.43</td>
<td>0.52</td>
<td>1.32</td>
<td>1.02</td>
<td>0.96</td>
</tr>
</tbody>
</table>
Conclusions

- First-principles theory of nuclear spin optical rotation has been formulated
- Experimental $^1$H rotation angles of liquid $\text{H}_2\text{O}(l)$ are quantitatively reproduced at the \textit{ab initio} CCSD level and at well-chosen DFT levels
- Optical chemical shift between similar nuclei in different chemical surroundings has been demonstrated
- Large NSOR predicted for $^{17}$O in liquid water
- Chemical distinction can be greatly enhanced by selective optical excitation of chromophores

Outlook

• Intermolecular interaction effects in Verdet constants and NSOR of H$_2$O(l) by combination of first-principles molecular dynamics simulation and the snapshot-supermolecule method
  [Pennanen, Ikäläinen, Lantto & JV, in preparation]

• Fully relativistic theory and calculations for $^{129}$Xe(l)
  [Ikäläinen et al., to be published]

• Experimental $^{17}$O NSOR in H$_2$O(l)
  [Romalis et al., to be published]
Acknowledgements

Science:
- M.Sc. Suvi Ikäläinen (Helsinki)
- Prof. Mike Romalis (Princeton)
- Doc. Perttu Lantto (Oulu)
- M.Sc. Teemu S. Pennanen (Oulu)

Money:
- Finnish Center of Excellence in Computational Molecular Science (CMS, 2006–11)
- National graduate school in Computational Chemistry and Molecular Spectroscopy
- Alfred Kordelin Fund (Suvi)
- Academy of Finland
International Master's Degree Programme at the University of Oulu, Finland:

Magnetic Resonance in Materials (MRM)

- Unique combination of experimental and computational education in nuclear magnetic resonance in various materials
- For BSc degree holders in physics, chemistry and materials science
- Language: English
- Application period: Jan 3rd – Feb 28th 2011, programme begins in autumn 2011, the norm completion time of MSc is two years
- Selection criteria: Bachelor's degree, sufficient background in physics, chemistry, mathematics and/or materials science (altogether at least 100 ECTS), sufficient proficiency in English
- Home page of the programme will be open in October 1st, see http://cc.oulu.fi/~nmrwww/mrm
- Project coordinator: Dr. Ville-Veikko Telkki (ville-veikko.telkki@oulu.fi)

- NMR Research Group of University of Oulu consists of experimental NMR and MR theory and computation sub-groups
- Group is a part of the Finnish Center of Excellence in Computational Molecular Science (CMS)
- The group has just received funding for three new, state-of-the-art NMR instruments
- Department of Physics is an official Centre of Excellence in Research within University of Oulu

\[
\sigma = \sigma_{\text{orb}} - \frac{\mu_B g \langle SS \rangle_0 \cdot A}{\gamma k T} \\
\langle SS \rangle_0 = \frac{\sum_{n} \langle n | SS | n \rangle \exp(-E_n(0)/kT)}{\sum_{n} \exp(-E_n(0)/kT)}
\]