

Chapter 1

Appendix A : Dipole-Dipole Hamiltonian

1.1 Derivation of the dipole-dipole Hamiltonian

The dipole-dipole interaction between two point-like magnetic dipoles can be derived classically by computing the static magnetic field generated by one dipole at the position of the second dipole.

For a magnetic dipole \mathbf{m} , positioned on $\mathbf{0}$, the static magnetic field generated on position $\mathbf{r} = r\mathbf{u}$ is : [1, p. 188]

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi} \left[\frac{3(\mathbf{m} \cdot \mathbf{u})\mathbf{u} - \mathbf{m}}{r^3} + \frac{8\pi}{3} \mathbf{m} \delta(\mathbf{r}) \right] \quad (1.1)$$

The interaction energy between two dipole \mathbf{m}_1 and \mathbf{m}_2 with relative position \mathbf{r} is therefore :

$$U = -\mathbf{m}_1 \cdot \mathbf{B}_2(\mathbf{r}) = -\frac{\mu_0}{4\pi} \left[\frac{3(\mathbf{m}_1 \cdot \mathbf{u})(\mathbf{m}_2 \cdot \mathbf{u}) - \mathbf{m}_1 \cdot \mathbf{m}_2}{r^3} + \frac{8\pi}{3} \mathbf{m}_1 \cdot \mathbf{m}_2 \delta(\mathbf{r}) \right] \quad (1.2)$$

The term in δ , which comes from the necessity to preserve $\nabla \cdot \mathbf{B} = 0$, is at the origin of the Fermi contact energy. This term plays a role for hyperfine coupling when there is an overlap of the electron wave-function with the nucleus, which is the case for s-orbitals in atoms. In the case of NV centers, Fermi contact energy plays an important role to the hyper-fine coupling between the NV^- electron spin and the nuclear spin of the ^{14}N or ^{15}N atom [2] or for nearby ^{13}C atoms [3].

However, in the scope of this manuscript, we will mostly concern ourselves with dipolar interaction between electronic spins separated by several atomic sites, so that the overlap of the electronic wave functions can be mostly neglected. This results in the simplified dipole-dipole coupling energy :

$$U = \frac{\mu_0}{4\pi} \left[\frac{\mathbf{m}_1 \cdot \mathbf{m}_2 - 3(\mathbf{m}_1 \cdot \mathbf{u})(\mathbf{m}_2 \cdot \mathbf{u})}{r^3} \right] \quad (1.3)$$

For two electronic spins, we can rewrite a quantized version of 1.3 by replacing the magnetic moments $\mathbf{m}_i = \hbar\gamma_i\hat{\mathbf{S}}_i$ where $\gamma_i = -\frac{g_e\mu_B}{\hbar}$ is the gyromagnetic

ratio of the electron. For the NV^- electronic spin, as well as most electronic spin defects in diamond, $g_e \approx 2$ which gives a numerical value for the gyro-magnetic ratio $\gamma \approx (2\pi) 28 \text{ GHz/T} \approx (2\pi) 2.8 \text{ MHz/G}$. $\hat{\mathbf{S}}_i = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$ is the spin vector operator for particle i . The quantized version of the dipole-dipole interaction is then:

$$\mathcal{H}_{dd} = \frac{J_0}{r^3} \left[\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 - 3(\hat{\mathbf{S}}_1 \cdot \mathbf{u})(\hat{\mathbf{S}}_2 \cdot \mathbf{u}) \right], \quad (1.4)$$

where $J_0 \equiv \frac{\mu_0 \gamma_1 \gamma_2 \hbar^2}{4\pi}$.

1.2 Decomposition of \mathcal{H}_{dd} over two different spin basis

Bibliography

- [1] John David Jackson. *Classical electrodynamics*. 1999.
- [2] MW Doherty et al. “Theory of the ground-state spin of the NV- center in diamond”. In: *Physical Review B* 85.20 (2012), p. 205203.
- [3] Benjamin Smeltzer, Lilian Childress, and Adam Gali. “ ^{13}C hyperfine interactions in the nitrogen-vacancy centre in diamond”. In: *New Journal of Physics* 13.2 (2011), p. 025021.