

394(8): Effect of the Vacuum on the Contact Term of NMR

By computer algebra:

$$\nabla \left(\frac{1}{r} \right) = -\frac{\underline{r}}{r^3} \quad (1)$$

$$= -\frac{(x\underline{i} + y\underline{j} + z\underline{k})}{(x^2 + y^2 + z^2)^{3/2}}$$

and

$$\nabla^2 \left(\frac{1}{r} \right) = -\frac{3}{r^3} + \frac{3\underline{r} \cdot \underline{r}}{r^5} = 0 \quad (2)$$

However, in contact theory:

$$\nabla^2 \left(\frac{1}{r} \right) = -4\pi \delta_D(r) \quad (3)$$

where

$$\delta_D(r) \neq 0 \quad (4)$$

is the Dirac delta function. The latter is also used in quantum mechanics, but clearly the contradiction between (2) and (3) means that $\delta_D(r)$ cannot be interpreted simply. At first, mathematicians dismissed the δ_D function as complete nonsense, but later, a new type of mathematics was developed to explain it.

In this note we bypass these difficulties with the MZ theory and the change of coordinate:

$$\underline{r} \rightarrow \underline{r} + \underline{\delta r} \quad (5)$$
$$= \underline{r}_1$$

Eq. (1) becomes:

$$\nabla \left(\frac{1}{|\underline{r} + \underline{\delta r}|} \right) = -\frac{(\underline{r} + \underline{\delta r})}{|\underline{r} + \underline{\delta r}|^3} \quad (6)$$

As in previous work:

$$|\underline{r} + \underline{\delta r}|^3 = \left(r^2 + 2\underline{r} \cdot \underline{\delta r} + \underline{\delta r} \cdot \underline{\delta r} \right)^{3/2}$$

$$= r^3 (1+x)^{3/2} \quad - (7)$$

where $x = \frac{1}{r^2} (2\underline{r} \cdot \underline{\delta r} + \underline{\delta r} \cdot \underline{\delta r})$ - (8)

So:

$$\nabla \left(\frac{1}{|\underline{r} + \underline{\delta r}|} \right) = - \frac{(\underline{r} + \underline{\delta r})}{r^3 (1+x)^{3/2}}$$

$$= - \frac{1}{r^3} (\underline{r} + \underline{\delta r}) \left(1 - \frac{3x}{2} + \frac{15}{8} x^2 + \dots \right) \quad - (9)$$

The isotropic average of this quantity can be evaluated. Using these methods, eq (2) in the presence of the vacuum becomes:

$$\nabla^2 \left(\frac{1}{r_1} \right) = - \frac{3}{r_1^3} + \frac{3 \underline{r}_1 \cdot \underline{r}_1}{r_1^5} \quad - (10)$$

$$= - \frac{3}{r^3 (1+x)^{3/2}} + \frac{3(\underline{r} + \underline{\delta r}) \cdot (\underline{r} + \underline{\delta r})}{r^5 (1+x)^{5/2}}$$

$$= - \frac{3}{r^3} \left(1 - \frac{3x}{2} + \frac{15}{8} x^2 + \dots \right) + \frac{3(\underline{r} + \underline{\delta r}) \cdot (\underline{r} + \underline{\delta r})}{r^5} \left(1 - \frac{5x}{2} + \frac{35}{8} x^2 + \dots \right)$$

$$\neq 0$$

The isotropic average $\langle \nabla^2 \left(\frac{1}{r_i} \right) \rangle$ can be worked out
by computer and the contact field is:

$$\underline{B}(\text{contact}) = -\frac{\mu_0 m}{4\pi} \langle \nabla^2 \left(\frac{1}{r_i} \right) \rangle \quad - (11)$$

This can be worked out $\neq 0$ to any order in ∞ .

Finally a theory of \underline{S}_R is used to model the
effect on the NMR spectrum.