1)

63(12): SUMMARY NOTE: Spin Connection for the Hartree Potential with Resonance.

The spin connection is a vector quantity $\underline{\omega}$ which can be either positive or negative. The spin connection for the Hartree potential is:

$$\underline{\omega} = \pm \frac{(\underset{\sim}{r} - \underset{\sim}{r}_i)}{|\underset{\sim}{r} - \underset{\sim}{r}_i|^2} \quad - (1)$$

for each electron or proton i.

1) Positive Spin Connection

$$\underline{E} = -\underline{\nabla}\phi = \underline{\omega}\phi \quad - (2)$$

$$\underline{\nabla} \cdot \underline{E} = \rho / \epsilon_0 . \quad - (3)$$

$$\underline{\omega} = \frac{\underset{\sim}{r} - \underset{\sim}{r}_i}{|\underset{\sim}{r} - \underset{\sim}{r}_i|^2} . \quad - (4)$$

2) Negative Spin Connection

$$\underline{E} = -\underline{\nabla}\phi = -\underline{\omega}\phi \quad - (5)$$

$$\underline{\omega} = -\frac{(\underset{\sim}{r} - \underset{\sim}{r}_i)}{|\underset{\sim}{r} - \underset{\sim}{r}_i|^2} \quad - (6)$$

Now denote:

$$\underset{\sim}{r} - \underset{\sim}{r}_i = (x - x_i)\,\underline{i} + (y - y_i)\,\underline{j} + (z - z_i)\,\underline{k} \quad - (7)$$

2)

So:

$$|\underset{\sim}{r} - \underset{\sim}{r}_i|^2 = (x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2 \quad - (8)$$

and:

$$\boxed{\underline{\omega} = \pm \frac{\left((x - x_i)\underline{i} + (y - y_i)\underline{j} + (z - z_i)\underline{k}\right)}{(x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2} \quad - (9)}$$

Therefore this is coded up into density functional code at each coordinate (x, y, z) of each electron and each proton of a molecule or lattice etc.

The Resonant Hartree Potential

1) Positive Spin Connection

$$\underline{E} = -\underline{\nabla}\phi + \underline{\omega}\phi \quad - (10)$$

where $\underline{\omega}$ is defined by the positive sign on the right hand side of eq. (9), i.e.

$$\underline{\omega} = \frac{\underset{\sim}{r} - \underset{\sim}{r}_i}{|\underset{\sim}{r} - \underset{\sim}{r}_i|^2} . \quad - (11)$$

2) Negative Spin Connection

$$\underline{\omega} = -\frac{(\underset{\sim}{r} - \underset{\sim}{r}_i)}{|\underset{\sim}{r} - \underset{\sim}{r}_i|^2} \quad - (12)$$

3)

Resonance Equation with Positive Spin Connection

$$\boxed{\nabla^2\phi - \frac{(\underset{\sim}{r}-\underset{\sim}{r}_i)}{|\underset{\sim}{r}-\underset{\sim}{r}_i|^2}\cdot\underline{\nabla}\phi + \frac{1}{|\underset{\sim}{r}-\underset{\sim}{r}_i|^2}\phi = -\frac{1}{\epsilon_0}\sum_{i=1}^{n} q_i\,\delta(\underset{\sim}{r}-\underset{\sim}{r}_i)} \quad -(13)$$

where $(\underset{\sim}{r}-\underset{\sim}{r}_i)/|\underset{\sim}{r}-\underset{\sim}{r}_i|^2$ is given by eq. (9) and where

$$|\underset{\sim}{r}-\underset{\sim}{r}_i|^{-2} = \left((x-x_i)^2+(y-y_i)^2+(z-z_i)^2\right)^{-1} \quad -(14)$$

In order to induce resonance the charge q_i must have an oscillatory character:

$$q_i = q_i(0)\cos(\underline{\kappa}\cdot\underline{r}) \quad -(15)$$

is the simplest type.

Resonance Equation with Negative Spin Connection

$$\boxed{\nabla^2\phi + \frac{(\underset{\sim}{r}-\underset{\sim}{r}_i)}{|\underset{\sim}{r}-\underset{\sim}{r}_i|^2}\cdot\underline{\nabla}\phi - \frac{1}{|\underset{\sim}{r}-\underset{\sim}{r}_i|^2}\phi = -\frac{1}{\epsilon_0}\sum_{i=1}^{n} q_i\,\delta(\underset{\sim}{r}-\underset{\sim}{r}_i)} \quad -(16)$$

Eqs (13) and (16) should be solved numerically and tested before being incorporated in density functional code packages.