## 63(9): The Spin Connection for the Hartree Potential

This is the vector:

$$\underline{\omega} = \frac{\underset{\sim}{r} - \underset{\sim}{r}'}{|\underset{\sim}{r} - \underset{\sim}{r}'|^3} \quad -(1)$$

From Jackson, page 25, eq. (1.2), 3rd ed. the force between two charges is:

$$\underline{F} = \frac{1}{4\pi\epsilon_0} e_1 e_2 \frac{\underset{\sim}{r}_1 - \underset{\sim}{r}_2}{|\underset{\sim}{r}_1 - \underset{\sim}{r}_2|^3} \quad -(2)$$

This is the force on a point charge $e_1$ located at $\underset{\sim}{r}_1$ due to another point charge $e_2$ located at $\underset{\sim}{r}_2$. The electric field at $\underset{\sim}{r}$ due to a point charge $e_1$ at $\underset{\sim}{r}_1$ is:

$$\underline{E}(\underset{\sim}{r}) = \frac{1}{4\pi\epsilon_0} e_1 \frac{(\underset{\sim}{r} - \underset{\sim}{r}_1)}{|\underset{\sim}{r} - \underset{\sim}{r}_1|^3} \quad -(3)$$

The electric field at $\underset{\sim}{r}$ due to a system of point charges $e_i$ at $\underset{\sim}{r}_i$, $i = 1, \ldots, n$ is the vector sum:

$$\underline{E}(\underset{\sim}{r}) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^{n} e_i \frac{(\underset{\sim}{r} - \underset{\sim}{r}_i)}{|\underset{\sim}{r} - \underset{\sim}{r}_i|^3} \quad -(4)$$

For each charge there is a spin connection:

2)

$$\underline{\omega}_i = \frac{\underset{\sim}{r} - \underset{\sim}{r}_i}{|\underset{\sim}{r} - \underset{\sim}{r}_i|^3} \quad -(5)$$

For computing purposes eq. (4) is preferred to the integral form:

$$\underline{E}(\underset{\sim}{r}) = \frac{1}{4\pi\epsilon_0} \int \rho(\underset{\sim}{r}') \frac{\underset{\sim}{r} - \underset{\sim}{r}'}{|\underset{\sim}{r} - \underset{\sim}{r}'|^3} d^3x' \quad -(6)$$

where:

$$\Delta q = \rho(\underset{\sim}{r}') \Delta x \Delta y \Delta z \quad -(7)$$

$$d^3x' = dx'\,dy'\,dz' \quad -(8)$$

but ~~the~~ integral form is used to derive ~~the~~ differential form of Coulomb's law:

$$\underline{\nabla} \cdot \underline{E} = \rho / \epsilon_0 . \quad -(9)$$

In special relativity (Maxwell Heaviside ~~theory~~):

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

where

$$\phi = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\underset{\sim}{r}')}{|\underset{\sim}{r} - \underset{\sim}{r}'|} d^3x \quad -(11)$$

3)

but in generally covariant unified field ~~theory~~:

$$\underline{E} = -\left(\underline{\nabla} + \underline{\omega}\right)\phi. \quad -(12)$$

In eq. (12) the sign of the spin connection has been chosen to be:

$$\underline{\omega} = -\frac{(\underset{\sim}{r} - \underset{\sim}{r}')}{|\underset{\sim}{r} - \underset{\sim}{r}'|^2} \quad -(13)$$

because this gives an undamped oscillator equation in exact form.

The resonant Hartree potential in 3-D is then defined by:

$$\boxed{\nabla^2\phi - \underline{\nabla}\cdot\left(\underline{\omega}\,\phi\right) = -\rho/\epsilon_0} \quad -(14)$$

If the spin connection is neglected eq (14) reduces to the Poisson equation:

$$\nabla^2\phi = -\rho/\epsilon_0 \quad -(15)$$

defining the Hartree potential $\phi$ of the standard model.

4) Eq. (14) is:

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

where:

$$\delta(\underset{\sim}{r} - \underset{\sim}{r}_i) = \delta(x_1 - X_1)\,\delta(y_1 - Y_1)\,\delta(z_1 - Z_1) \quad -(17)$$

is the three dimensional Dirac delta function.

The charge density is defined by:

$$\rho(\underset{\sim}{r}) = \sum_{i=1}^{n} e_i \, \delta(\underset{\sim}{r} - \underset{\sim}{r}_i) \quad -(18)$$

Incorporation into Density Functional Code

The resonant Hartree potential $\phi$ from eq. (16) can be incorporated directly ~~from~~ into density functional code, or eq. (16) can be further reduced to an undamped oscillator

5) equation because eq. (16) is an example of an Euler equation in three dimensions. It may be written as:

$$|\underset{\sim}{r}-\underset{\sim}{r}_i|^2 \nabla^2 \phi + (\underset{\sim}{r}-\underset{\sim}{r}_i)\cdot \underline{\nabla}\phi - \phi = -\frac{|\underset{\sim}{r}-\underset{\sim}{r}_i|^2}{\epsilon_0} \sum_{i=1}^{n} e_i \delta(\underset{\sim}{r}-\underset{\sim}{r}_i) \quad -(19)$$

Now use:

$$|\underline{r}-\underset{\sim}{r}_i|^2 = (\underset{\sim}{r}-\underset{\sim}{r}_i)\cdot(\underset{\sim}{r}-\underset{\sim}{r}_i) \quad -(20)$$

and denote:

$$\underline{R}_i := \underset{\sim}{r}-\underset{\sim}{r}_i. \quad -(21)$$

So eq. (19) is:

$$(\underline{R}_i\cdot\underline{R}_i)\nabla^2\phi + \underline{R}_i\cdot\underline{\nabla}\phi - \phi = -(\underline{R}_i\cdot\underline{R}_i)\frac{\rho}{\epsilon_0}. \quad -(22)$$

Now let

$$\underline{R}_i\cdot\underline{R}_i = x^2+y^2+z^2 \quad -(23)$$

$$\underline{R}_i\cdot\underline{\nabla}\phi = x\frac{\partial\phi}{\partial x} + y\frac{\partial\phi}{\partial y} + z\frac{\partial\phi}{\partial z} \quad -(24)$$

for each charge $i = 1, \ldots, n$.

6)

Then:

$$(x^2+y^2+z^2)\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}\right)$$
$$+x\frac{\partial\phi}{\partial x}+y\frac{\partial\phi}{\partial y}+z\frac{\partial\phi}{\partial z}-\phi$$
$$=-(x^2+y^2+z^2)\frac{\rho_0}{\epsilon_0}\cos(\underline{\kappa}\cdot\underline{r}) \quad -(25)$$

where:

$$\rho := \rho_0\cos(\underline{\kappa}\cdot\underline{r})$$
$$=\rho_0\cos(\kappa_x x+\kappa_y y+\kappa_z z) \quad -(26)$$

If:

$$\underset{\sim}{r} = Z\underline{k} \quad -(27)$$

eq. (26) reduces to eq. (14) of notes 63(9).

We may now reduce eq. (25) to an undamped oscillator, or alternatively solve it numerically. The reduction will be the next stage of the calculation.