1) 60(9): Perturbation Method

Standard Model

The H atom in the standard model is given by:

$$\hat{H}\psi = E\psi \quad -(1)$$

i.e.:

$$-\frac{\hbar^2}{2m}\nabla^2\psi = (E - V)\psi \quad -(2)$$

where

$$V = -e\phi, \quad \phi = \frac{e}{4\pi\epsilon_0 r}. \quad -(3)$$

The potential is given by:

$$\underline{E} = -\underline{\nabla}\phi, \quad \underline{\nabla}\cdot\underline{E} = \rho/\epsilon_0. \quad -(4)$$

ECE Theory

The potential ϕ is given by:

$$\nabla^2\phi + (\underline{\nabla}\cdot\underline{\omega})\phi + \underline{\omega}\cdot\underline{\nabla}\phi = -\rho/\epsilon_0 \quad -(5)$$

i.e.:

$$\boxed{\nabla^2\phi = -\rho/\epsilon_0 - \underline{\nabla}\cdot(\underline{\omega}\phi).} \quad -(6)$$

In the standard model, eq. (6) is:

$$\nabla^2\phi = -\rho/\epsilon_0, \quad -(7)$$

the Poisson equation. So the effect of a spin connection $\underline{\omega}$ is to add a charge density:

$$\boxed{\rho_1 = \epsilon_0\underline{\nabla}\cdot(\phi\underline{\omega})} \quad -(8)$$

2)

In the first approximation, ϕ in eq. (8) may be taken to be the Coulombic potential:

$$\phi_c = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\underset{\sim}{r}')}{|\underset{\sim}{r} - \underset{\sim}{r}'|} d^3r' \quad -(9)$$

so:

$$\rho_1 \sim \underline{\nabla} \cdot \left(\frac{\underline{\omega}}{4\pi} \int \frac{\rho(\underset{\sim}{r}')}{|\underline{r} - \underline{r}'|} d^3r' \right) \quad -(10)$$

where $\rho(\underset{\sim}{r}')$ is the Coulombic charge density used in density functional code for the H atom.

Therefore:

$$\boxed{\nabla^2 \phi \sim -\frac{1}{\epsilon_0} (\rho + \rho_1)} \quad -(11)$$

and

$$\phi \sim \frac{e_1}{4\pi\epsilon_0 r} \quad -(12)$$

where e_1 is an effective or perturbed charge.

At resonance, ϕ from eq. (6) becomes very large, and this can be thought of as $\underset{\sim}{r} \rightarrow \underset{\sim}{r}'$ in eq. (10), although a perturbation method is not valid when ϕ is very la