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Qunatum Chemistry in view of Riemann Space

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Let us review the quantum chemistry in view of Riemann geometry or in the general relativity. The theory has the flamework of space(coordinate) and object. In the general relativity the distinction between these is lost. The quantun theory is the theory in Hilbert space. the usual space-time is parameter and the physical object is operator.

Some similarity will be expected between the bond order and the metric of Riemann space. Discussin begins with what vacuum is. We state that vacuum seems to imply the ground state, precisely speaking, the condensed state of many particles.

1. If the gravitaion is quantized, graviton shold be boson, so that the infinite number of graviton condense in the single level at $T = 0$. The wave function function of graraviton should be similar to the Klein-Gordon equation.

2. On the other hand the elctron is fermion, of which wave function is Schrödinnger function. The single elctron is restricted to occupy the single level.

   We assume that the ground state of gravitons is characterized by metrices $g_{\mu\nu}$, $\mu, \nu = 0 \sim 3$. The elememt $g_{\mu\nu} = \mathbf{n}_\mu \cdot \mathbf{n}_\nu$ is the scalar product of the basic vectors $\mathbf{n}_\mu$. These are considerd to be the wave functions in the quantum mechanical sense. In vacuum,

   $$g_{\mu\nu} = diag(1 \ -1 \ -1 \ -1) \tag{1}$$

3. The quantity of the electronic system corresponding to $g_{\mu\nu}$ might be the bond order, q_{rs} where r, s are site indices.

   The Hamiltonian presents the structure of model for molecule; for butadine in the Hückel model,

   $$\begin{aligned} H &= |r > \beta_{rs} < s| \qquad (r, s = 1 \sim 4) \\ &= \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & -1 & 0 \\ 0 & -1 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \end{aligned} \tag{2}$$

   where the unit $\beta_{rs} = -1$ for simplicity. Solving this eigen value problem, we have the eigen functios, so that, the bond order matrix is obtained as

   $$q_{rs} = \begin{pmatrix} 1.000 & .894 & .000 & -.447 \\ .894 & 1.000 & .447 & .000 \\ .000 & .447 & 1.000 & .894 \\ -.447 & .000 & .894 & 1.000 \end{pmatrix} \tag{3}$$

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It is important to note that the coupling terms of Hamiltoian is restricted to nearest neibours, while the bond order is extended over the system. The bond order is really the order of the system.

4. In general relativity, the space-time is Riemsnnian, so that the distance is given in the oblique coordinate with metric,

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu \tag{4}$$

and the equation of motion is

$$
\begin{aligned}
\frac{d^2 u^\mu}{ds^2} + \Gamma^\mu_{\nu\rho}\frac{du^\nu}{ds}\frac{du^\rho}{ds} &= 0 \\
\frac{du^\mu}{ds} + \Gamma^\mu_{\nu\rho}\lambda^\nu\frac{du^\rho}{ds} &= 0 \qquad \lambda^\mu = \frac{du^\mu}{ds}
\end{aligned}
\tag{5}
$$

wher $\Gamma^\mu_{\nu\rho}$ is the Christoffel, and s is the world time. Similarity between $g_{\mu\nu}$ and q_{rs} is pointed out.

5. Define the covaeint derivarive,,

$$ A_{\mu:\nu} = A_{\mu,\nu} - \Gamma^\alpha_{\mu\nu}A_\alpha \tag{6}$$

so it

$$
\begin{aligned}
g_{\mu:\nu} &= g_{\mu,\nu} - \Gamma^\alpha_{\mu,\nu}g_{\alpha,\nu} - \Gamma^\alpha_{\mu\nu}g_{\mu\alpha} \\
&= g_{\mu,\nu} - \Gamma_{\mu,\nu\alpha} - \Gamma^\alpha_{\mu\nu\mu\alpha} \\
&= 0
\end{aligned}
\tag{7}
$$

say, $g_{\mu\nu}$ is vanishing for the covarint derivative. It is seen that $\Gamma_{\mu,\nu\alpha}$ reflects the structure of the space-time. The gauge potential is deeply relsted with this.

6. In order to investigate the structure of space-time, in the general relatity, the Ritti tensor R is introduced. The condition,

$$ R_{\mu\nu} = 0 \tag{8}$$

tells us that the space-time is flat, and this condition is reduce to

$$ g_{\alpha'\beta',\nu}\, x^{\alpha'}_\mu x^{\beta'}_\lambda = 0 \quad \text{or} \quad g_{\alpha'\beta',\nu} = 0 \tag{9}$$

7. Then $q_{rs,mn} \to 0$ imply the molecule is flat ?