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Electronic stress tensor of chemical bond

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Electronic stress tensor of chemical bond $\overleftrightarrow{S}$ is a 3-dim real symmetric component of a 3-dim real stress tensor $\overleftrightarrow{\Pi}$. The complementary antisymmetric component $\overleftrightarrow{A} = \overleftrightarrow{\Pi} - \overleftrightarrow{S}$ drives the torque of electron spin $\vec{s}$ through the vorticity $\mathrm{rot}\vec{s}$. The whole picture has quite recently been unified on the variation principle of gravity using the semiclassical action integral. This theory is extended in this paper using a quantum action integral based on a simple SUGRA (supergravity), which is a simple SUSY (supersymmetry) model of gravity.

Keywords: Stress tensor, Electronic stress tensor, Energy density, Semiclassical action integral, Quantum action integral

Recently, we have developed the concept of energy density using the stress tensor of QED (quantum electrodynamics).[1-5] The symmetrical component $\overleftrightarrow{S}$ of the electronic stress tensor has been proved to predict the emergence of the covalent bond in terms of the spindle structure.[4] The theory of the spindle structure has also been developed to visualize the regional chemical potential of chemical reactivity and the bond order of chemical bond.[6-11]

The energy density concept itself has been essential in the quantum field theory and the stress tensors are used ubiquitously for description of internal forces of matter. They have been originally formulated by Pauli[12] in the quantum mechanical context with the differential force law showing that it can be derived from the divergence relations applied to the energy-momentum tensor under general situations in the presence of electromagnetic fields, while the basic idea dates back to Schrödinger.[13]

We have also found a new picture of electron spin torque, where the chirality of the electronic structure has played an essential important role.[5,8] The theory of the electron spin torque has also been developed to visualize the chirality characteristics of atoms and chiral molecules.[14-16]

Quite recently, the concept of energy density has been formulated in terms of stress tensor in general relativity.[17-19] The spin vorticity of electron $\mathrm{rot}\vec{s}$ has been hidden in the energy-momentum tensor and plays a significant role in the dynamics of electron. The dynamics of electron spin is driven by the antisymmetric component of the stress tensor of electron through the vorticity. The symmetric component of the stress tensor of electron drives the tensorial energy density of chemical reactivity. The whole picture of the electronic stress tensor has been established on the variation principle of gravity using the semiclassical action integral.[17-19]

In this paper, this theory is extended, following a short review of the preceding papers, using a quantum action integral based on a simple SUGRA (supergravity), which is a simple SUSY (supersymmetry) model of gravity. To make the paper self-contained, fundamental mathematics[17-21] are collected in Appendices SA-SD (see Supplementary Data).

Stress Tensor

The Dirac equation of the Dirac spinor with the covariant derivative D of QED is given as Eqs (1) and (2),

$$\left(i\hbar\Gamma D - mc\right) = 0 \qquad \ldots (1)$$

$$D = \partial + i\frac{q}{\hbar c}A \qquad \ldots (2)$$

where m is the mass of electron, c is the speed of light in vacuum, $q = -e$ is the charge of electron and A is the Abelian gauge potential of photon.

The kinetic momentum density $\vec{\Pi}$ defined as Eq. (3),

$$\vec{\Pi} = \frac{1}{2}\left({}^{\dagger}\left(i\hbar\vec{D}\right) + h.c.\right) \qquad \ldots (3)$$

satisfies the equation of motion with the force density in the right hand side of Eq. (4),

$$\frac{\partial}{\partial t}\vec{\Pi} = \vec{L} + {}^{\rightarrow\Pi} \qquad \ldots (4)$$

The force density is composed not only of the Lorentz force density $\vec{L}$, but also of the tension density ${}^{\rightarrow\Pi}$ which is the divergence of the 3-dim real stress tensor ${}^{\leftrightarrow\Pi}$ Eqs (5) and (6).

$${}^{\rightarrow\Pi} = \mathrm{div}\,{}^{\leftrightarrow\Pi}, \quad {}^{\rightarrow\Pi k} = \partial_{\ell}\ {}^{\Pi k\ell} \qquad \ldots (5)$$

$${}^{\Pi} = \frac{c}{2}\left({}^{-}\Gamma \left(-i\hbar D\ \right) \ + h.c.\right) \qquad \ldots (6)$$

The stress tensor itself is not defined uniquely since mathematically any tensor whose divergence is zero can be added to. The stress tensor ${}^{\leftrightarrow\Pi}$ in Eq. (6) is defined in such a way that it appears in the equation of motion of $\vec{\Pi}$ as in Eq. (4).

Variation principle and the spin connection

To seek for the variation principle of the equation of motion, the semiclassical Einstein-Hilbert action integral has been used under the symmetry of the general coordinate transformation of gravity (Eq. 7),

$$\Delta I = 0, \quad I = \frac{c}{2}\int R\sqrt{-g}\,d^4x + \frac{1}{c}\int L\sqrt{-g}\,d^4x, \qquad \ldots (7)$$
$$= \frac{8\Pi G}{c^2}$$

where R is the Ricci scalar, G is the universal gravitational constant and L is the Lagrangian density of QED including the interaction with gravity.

The gravitational covariant derivative $D\ (g)$ is then given as Eq. (8),

$$D\ (g) = \partial\ + i\frac{q}{\hbar c}A\ + + i\frac{1}{2\hbar}\Gamma_{ab}\ J^{ab} \qquad \ldots (8)$$
$$= D\ + i\frac{1}{2\hbar}\Gamma_{ab}\ J^{ab}$$

with the spin angular momentum J^{ab} as Eq. (9),

$$J^{ab} = \frac{i\hbar}{4}\left[\Gamma^{a}, \Gamma^{b}\right] \qquad \ldots (9)$$

and spin connection as Eq. (10).

$$\Gamma_a^{b}\ = e_{a\ ;}\ {}^{bc}e_c \qquad \ldots (10)$$

Using the gravitational covariant derivative $D\ (g)$, the stress tensor of electron ${}^{\Pi}\ (\mathrm{g})$ becomes Eq. (11).

$${}^{\Pi}\ (\mathrm{g}) = \frac{c}{2}\left({}^{-}\Gamma \left(-i\hbar D\ (g)\right) \ + h.c.\right) \qquad \ldots (11)$$

In this variation principle, due to the presence of the spin connection Γ_{ab}, a new symmetry-polarized geometrical tensor ${}^{\Pi}$ appears and whose antisymmetric component cancels with that of ${}^{\Pi}\ (g)$ (Eq. 12),

$${}^{A}\ + {}^{A}\ (g) = 0 \qquad \ldots (12)$$

where

$${}^{A}\ = \frac{1}{2}\left({}^{\Pi}\ - {}^{\Pi}\ \right) \qquad \ldots (13)$$

$${}^{A}\ (g) = \frac{1}{2}\left({}^{\Pi}\ (g) - {}^{\Pi}\ (g)\right) \qquad \ldots (14)$$

Symmetry of the stress tensor with spin vorticity

This cancellation ${}^{A}\ + {}^{A}\ (g) = 0$ (Eq. 12), originates from the fact that in order to satisfy the symmetry under the general coordinate transformation, the energy-momentum tensor T should be symmetric (Eq.15).

$$T\ = T \qquad \ldots (15)$$

It follows that the electronic part of the energy-momentum tensor T_{e} of T should be symmetric Eq. (16).

$$T_{\mathrm{e}}\ = -\ {}^{\Pi}\ -\ {}^{\Pi}\ (g) = T_{\mathrm{e}} \qquad \ldots (16)$$

Consequently, the cancelling equation ${}^{A}\ + {}^{A}\ (g) = 0$ (Eq. 12), is mandatory. It has the physical meaning, which in the limit to the Minkowski spacetime turns out to be two-fold; the time-like change of spin, namely the equation of motion of spin $\vec{s}$ with torque $\vec{t}$ and zeta force $\vec{\ }$ (Eq. 17),

$$\frac{\partial}{\partial t}\vec{s} = \vec{t} + \vec{\ } \qquad \ldots (17)$$

and the space-like change of spin, namely, the spin vorticity (Eq. 18).

$$\mathrm{rot}\vec{s} = \frac{1}{2}\left({}^{-}\Gamma\left(i\hbar D_0\right) \ + h.c.\right) - \vec{\Pi} \qquad \ldots (18)$$

Thus, in the limit to the Minkowski spacetime, the equation of motion of electron, Eq. (4), is reduced to

$$\frac{\partial}{\partial t}\left(\vec{\Pi}+\frac{1}{2}\mathrm{rot}\vec{s}\right)=\vec{L}+\ ^{\to S} \qquad \ldots (19)$$

$$^{\to S}=\mathrm{div}\ ^{\leftrightarrow S}, \quad ^{\to Sk}=\partial_{\ell}\ ^{Sk\ell} \qquad \ldots (20)$$

$$^{S}\ =\frac{1}{2}\left(\ ^{\Pi}\ +\ ^{\Pi}\ \right) \qquad \ldots (21)$$

It should be noted that half the vorticity, $\frac{1}{2}\mathrm{rot}\vec{s}$ appears as a component of the electronic momentum, as found in Eq. (19). Also, this assures the equation of motion of electron using solely the symmetric part of the tensor $^{S}_{k\ell}$ in the right hand side.

The SUGRA spin connection and the symmetry of the stress tensor

In the tetrad formalism, the Dirac spinor field is a coordinate scalar and a Lorentz spinor.

$$(x)\to\ '\ (x')=\ (x) \qquad \ldots (22)$$

$$(x)\to\ '(x)=D\left(\Lambda(x)\right)\ (x) \qquad \ldots (23)$$

Also, what is important is that the covariant derivative $D\ (g)$ is not only a coordinate scalar, but also a Lorentz vector.

$$D\ (g)=\partial\ +\Gamma \qquad \ldots (24)$$

$$\Gamma\ (x)\to\Gamma\ '(x)=D(\Lambda(x))\Gamma\ (x)D^{-1}(\Lambda(x)) - \left(\partial\ D(\Lambda(x))\right)D^{-1}(\Lambda(x)) \qquad \ldots (25)$$

The spin connection is not unique. In SUGRA, we have a new term $\Gamma_{ab}\ (\mathrm{SUGRA})$ added to Γ_{ab} (Eq.26).

$$\begin{aligned} D\ (\mathrm{SUGRA}) &= \partial\ +i\frac{q}{\hbar c}A\ ++i\frac{1}{2\hbar}\Gamma_{ab}\ J^{ab} \\ &\quad +i\frac{1}{2\hbar}\Gamma_{ab}\ (\mathrm{SUGRA})J^{ab} \\ &= D\ (g)+i\frac{1}{2\hbar}\Gamma_{ab}\ (\mathrm{SUGRA})J^{ab} \end{aligned} \qquad \ldots (26)$$

Then the symmetry-polarized stress tensor of electron $^{\Pi}\ (\mathrm{g})$ is changed to $^{\Pi}\ (\mathrm{SUGRA})$ with the covariant derivative $D\ (\mathrm{SUGRA})$ (Eq. 27).

$$(\mathrm{SUGRA})=\frac{c}{2}\left(\ ^{-}\Gamma\left(-i\hbar D\ (\mathrm{SUGRA})\right)\ +h.c.\right) \qquad \ldots (27)$$

With the new spin connection term given, the new symmetry-polarized geometrical tensor $^{\Pi}\ (\mathrm{SUGRA})$ appears, and again now that the energy-momentum tensor $T\ (\mathrm{SUGRA})$ is symmetric, and hence the electronic part $T_{\mathrm{e}}\ (\mathrm{SUGRA})$ is symmetric, the resultant antisymmetric component of the $^{A}\ (\mathrm{SUGRA})$ cancels with $^{A}\ (\mathrm{SUGRA})$:

$$^{A}\ (\mathrm{SUGRA})+\ ^{A}\ (\mathrm{SUGRA})=0 \qquad \ldots (28)$$

where

$$^{A}\ (\mathrm{SUGRA})=\frac{1}{2}\left(\ ^{\Pi}\ (\mathrm{SUGRA})-\ ^{\Pi}\ (\mathrm{SUGRA})\right) \qquad \ldots (29)$$

$$^{A}\ (\mathrm{SUGRA})=\frac{1}{2}\left(\ ^{\Pi}\ (\mathrm{SUGRA})-\ ^{\Pi}\ (\mathrm{SUGRA})\right) \qquad \ldots (30)$$

Examples of symmetric energy-momentum tensor

We shall examine an example of the symmetric energy-momentum tensor of a simple SUGRA in the case of a simple SUSY with linearized gravity.

A weak classical gravity is represented by the infinitesimal transformation[20]

$$x\ (x)\to x'\ (x)=x\ (x)+\Xi\ (x) \qquad \ldots (31)$$

$$\Lambda^{a}{}_{b}(x)\to\Lambda'^{a}{}_{b}(x)=\Delta^{a}{}_{b}+\ ^{a}{}_{b}(x) \qquad \ldots (32)$$

$$\begin{aligned} e^{a}\ (x) &= \Delta^{a}\ +2k\ ^{a}\ (x)\to e'^{a}\ (x') \\ &= \Delta^{a}\ +2k\ '^{a}\ (x') \end{aligned} \qquad \ldots (33)$$

$$(x)\to\ '\ (x')=\ (x) + \frac{1}{2k}\left(-\frac{\partial\Xi\ (x)}{\partial x}+\ (x)\right) \qquad \ldots (34)$$

where

$$k=\sqrt{8\Pi G}\frac{\hbar}{c^{2}} \qquad \ldots (35)$$

This leads to a weak gravitational field $h\ (x)$ Eqs (36) and (37).

$$g\ (x)=\ +2kh\ (x) \qquad \ldots (36)$$

$$h\ (x)=\ (x)+\ (x) \qquad \ldots (37)$$

The action integral given in Eq. (7) is cast into the linearized form as follows:

$$I=\frac{c}{2}\int R\sqrt{-g}d^{4}x+\frac{1}{c}\int L\sqrt{-g}d^{4}x \xrightarrow{\text{linearized}}$$

$$I_{\text{linearized}}=\frac{1}{c}\int d^{4}x\left(-\hbar^{2}E\ \ h\ \ -kT\ \ h\ \ +L^{(0)}{}_{\text{linearized}}\right) \qquad \ldots (38)$$

$$E \quad = \frac{1}{2}\begin{pmatrix} \Box h \quad -\partial \, \partial \, h \quad -\partial \, \partial \, h \\ +\partial \, \partial \, h \quad - \quad \Box h \quad + \quad \partial \, \partial \, h \end{pmatrix} \quad \ldots (39)$$
$$= E$$

where E is the linearized Einstein tensor and $L^{(0)}_{\text{linearized}}$ is the linearized Lagrangian density of QED excluding the interaction with gravity. In the right hand side of Eq. (38), we have the symmetric energy-momentum tensor $T \quad = T$, and hence the symmetric stress tensor $T_{\text{e}} \quad = T_{\text{e}}$ as the electronic part.

In SUGRA, we have the gauge transformation of the spin-2 field of graviton $h \quad (x)$ (Eq. 40).

$$h \quad (x) \to h' \quad (x) = h \quad (x) - \frac{1}{2k}\left(\frac{\partial \Xi \, (x)}{\partial x} + \frac{\partial \Xi \, (x)}{\partial x}\right) \quad \ldots (40)$$

The graviton is associated with the superpartner, called the gravitino $\quad (x)$, represented by the spin-3/2 Rarita-Schwinger field, whose gauge transformation is (Eq. 40),

$$(x) \to \quad ' \, (x) = \quad (x) - \partial \quad (x) \quad \ldots (41)$$

where $\quad (x)$ is a spin-1/2 Majorana field. These are the components of the metric superfield $H \quad (x)$, whose gauge transformation is given by Eq. (42),

$$H \quad (x) \to H' \quad (x) = H \quad (x) - \Delta \quad (x) \quad \ldots (42)$$

where $\Delta \quad (x)$ is the linear superfield (Eq. 43).

$$\Delta \quad (x) = \bar{d}\,\Xi(x)\,\Gamma \quad \ldots (43)$$

The gauge fields are then calculated to be

$$(x) = V^{H} \quad (x) - \frac{1}{3} \quad V^{H\Lambda}{}_{\Lambda}(x) \quad \ldots (44)$$

$$(x) = 2\Lambda^{H} \quad (x) - \frac{2}{3}\,\Gamma \,/\!\!\!\Lambda^{H}(x) + \frac{2}{3} i\hbar \;\, \Gamma\partial \quad {}^{H} \quad (x) \quad \ldots (45)$$

with

$$\Xi \, (x) = 2kv \quad (x) \quad \ldots (46)$$

$$v \quad (x) = -\hbar^{-\Xi}(x)\,\Gamma + \text{const} \quad \ldots (47)$$

$$(x) = k\left(\partial \; v \quad (x) - \partial \; v \quad (x) - V^{\Delta} \quad (x) + V^{\Delta} \quad (x)\right) \quad \ldots (48)$$

$$(x) = 4i\hbar M^{\;\Xi}(x) - 4\hbar\Gamma_5 N^{\;\Xi}(x) + \text{const} \quad \ldots (49)$$

Consequently, the gauge-invariant linearized SUGRA action integral is found to be

$$I_{\text{linearized}}(\text{SUGRA})$$
$$= I_{\text{linearized}} - \frac{1}{c}\int d^4x \begin{pmatrix} \frac{1}{2} - \; L \; \times c - \frac{1}{2} k\hbar^{-1}\bar{S}_{new} \\ -\frac{4}{3}\left(b \;\, b \; + 2p^2 + 2s^2\right) \\ +k\hbar^{-1}\left(-R \;\, b \; + 2pA^{X} - 2sB^{X}\right) \end{pmatrix} \quad \ldots (50)$$

where S_{new} is the supersymmetry current, and

$$R \quad = 2C^{\Theta} \quad \ldots (51)$$

is the R-current, and

$$L \quad = -\frac{\hbar}{c} \qquad \partial \;\, \Gamma_5 \, \Gamma \quad \ldots (52)$$

$$b \quad = D^{H} \; - \hbar^2 \partial \; \partial \; C^{H} \; + \frac{1}{2}\hbar \qquad \partial \; V^{H} \quad \ldots (53)$$

$$p = i\hbar\partial \;\; N^{H} \quad \ldots (54)$$

$$s = i\hbar\partial \;\; M^{H} \quad \ldots (55)$$

Further optimization of the auxiliary fields b, p, and s leads to Eq. (56)

$$I_{\text{linearized}_{opt}}(\text{SUGRA}) =$$
$$I_{\text{linearized}} - \frac{1}{c}\int d^4x \begin{pmatrix} \frac{1}{2} - \; L \; \times c - \frac{1}{2} k\hbar^{-1}\bar{S}_{new} \\ +\frac{3}{8}k^2\hbar^{-2}\begin{pmatrix} \frac{1}{2} R \;\; R \\ +\left(A^{X}\right)^2 + \left(B^{X}\right)^2 \end{pmatrix} \end{pmatrix} \quad \ldots (56)$$

We may identify the negative energy density, $-\frac{3}{8}k^2\hbar^{-2}\left(\left(A^{X}\right)^2 + \left(B^{X}\right)^2\right)$, for the anti-de Sitter spacetime.

We have the SUGRA action added to $I_{\text{linearized}}$, as shown in Eqs (50) and (56), so that we have again the symmetric energy-momentum tensor $T \quad = T$, and hence the symmetric stress tensor $T_{\text{e}} \quad = T_{\text{e}}$ as the electronic part.

Conclusions

We have extended the theory of the electronic stress tensor of chemical bond on the variation principle of gravity using the semiclassical action integral to the one using a quantum action integral. The central symmetrical properties of the theory have shown to be intact. Further characteristics of the supersymmetry[20] may play a significant role in the theory of the electronic stress tensor of chemical bond.

Supplementary Data

Supplementary Data associated with this article, i.e., Appendices SA-SD, are available in the electronic form at http://www.niscair.res.in/jinfo/ijca/IJCA_53A (8-9)1031-1035_SupplData.pdf.

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