3P119

H_2^+ 分子のストレステンソルによる解析

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The stress tensors are used widely for description of internal forces of matter. For some time it is also applied in quantum theory in studies of molecular properties in chemical systems. Electronic stress tensors measure effects caused by internal forces acting on electrons in molecules and particularly those between bonded atoms [1]. It has been proposed to define stress tensor originated bond orders expressing bond strengths in terms of these internal forces [2].

Here, we elucidate the role of electronic stress tensor in a one-electrom molecule using H_2^+ whose exact wavefunctions are known [3]. Stress tensor τ^S for the wavefucntion ψ is constructed as

$$\tau_{kl}^S = \frac{\hbar^2}{4m}\left(\psi^*\partial_k\partial_l\psi - \partial_k\psi^*\partial_l\psi + \partial_k\partial_l\psi^* \cdot \psi - \partial_l\psi^*\partial_k\psi\right), \tag{1}$$

and its trace gives the energy density. The distribution of the largest eigenvalue and its eigenvector is plotted in Fig. 1 for the ground state. We can define bonding region by the one with positive largest eigenvalues of stress tensor which indeed spreads between H atoms. The bond strength may be defined by integrating energy density within such a bonding region.

参考文献

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[2] P. Szarek and A. Tachibana, *J. Mol. Model* **13** 651 (2007).

[3] K. Ichikawa and A. Tachibana, *in preparation.*

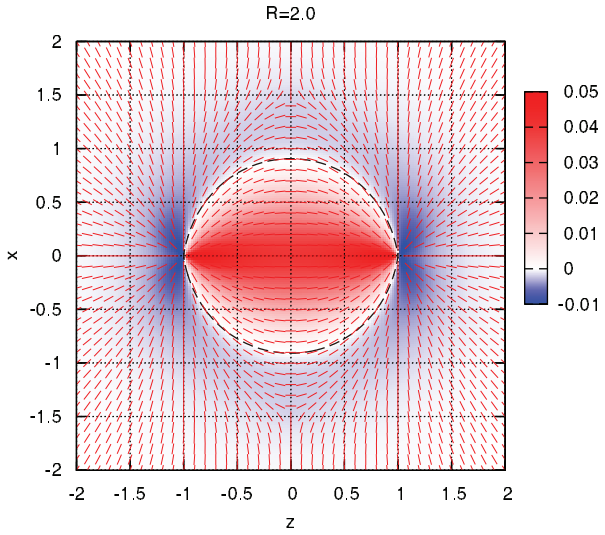

図 1: The spatial distribution of the largest eigenvalue of stress tensor of H_2^+ molecule is plotted in the plane including two H atoms. They are located at $(z, x) = (-1.0, 0.0)$ and (1.0, 0.0). The dashed line shows the zero surface of the eigenvalue and it is positive inside the circle and is negative outside. Also shown are corresponding eigenvectors. Atomic units are used.