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Note

About a Relation Between Slater and Gaussian Functions

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Using the generating function of Hermite polynomials a relation between Slater and Gaussian functions is presented, which formally can be interpreted as the inverse of the integral transformation used by Shavitt and Karplus.

In 1954 Kikuchi[1] has shown, how Slater and Gaussian functions can be connected by an integral transform formula which later was widely used by Shavitt and Karplus[2] in their computations

$$S\,(a, r) = a/(2\pi^{1/2}) \int_{o}^{\infty} dt\, t^{-3/2}\, e^{-a^2/(4t)}\, G\,(t, r)$$

where

$$S\,(a, r) = e^{-ar} \quad \text{and} \quad G\,(t, r) = e^{-tr^2}$$

As an approximation of the above relation we can mention the small Gaussian expansion of Slater type orbitals using the least squares fit method[3,4]. The expansion is not unique, nevertheless conceptually it is a very simple approach and is extensively used in *ab initio* computations of molecular properties.

The aim of the present short communication is to report on another relation which can be established between Slater and Gaussian orbitals using the generating function of Hermite polynomials[5]

$$e^{2xz - z^2} = \sum_{n=o}^{\infty} H_n\,(x)\, z^n/n!$$

where $H_n\,(r)$ is a Hermite polynomial of order n

$$H_n\,(r) = (-)^n\, e^{r^2}\, D_r^n\, e^{-r^2} \quad \text{and} \quad D_r = d/dr$$

By making substitutions $z = rt^{1/2}$, $x = a/(2\, t^{1/2})$ and using the property $D_a S\,(a, r) = -\, rS\,(a, r)$ of the Slater functions in the expression of the generating function, the following relation can be observed between Slater and Gaussian orbitals

$$G\,(t, r) = Q\,(t, a)\; S\,(a, r)$$

where

$$Q\,(t, a) = \sum_{n=o}^{\infty} (-)^n\, t^{n/2}/n!\; H_n\,(a/(2t^{1/2}))\; D_a^n$$

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The »operator« Q presented here may be helpful in studying quantitative differences between Slater and Gaussian type orbitals.

In conclusion the following symbolic relations can be written

$$(\text{SLATER}) = (\text{SHAVITT-KARPLUS}) \times (\text{GAUSS})$$
$$(\text{GAUSS}) = (\text{GENERATING-HERMITE}) \times (\text{SLATER})$$

where the meaning of the symbols is self-explanatory.

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REFERENCES

1. R. Kikuchi, *J. Chem. Phys.* **22** (1954) 148.
2. I. Shavitt and M. Karplus, *J. Chem. Phys.* **36** (1962) 550.
3. K. O-Ohata, H. Taketa, and S. Huzinaga, *J. Phys. Soc. Japan* **21** (1966) 2306.
4. R. F. Stewart, *J. Chem. Phys.* **52** (1970) 431.
5. A. Erdélyi, (Editor), *Higher Transcendental Functions,* Vol. 2, p. 194, McGraw--Hill, Co. Inc., New York, 1953.

IZVOD

Veza Slaterovih i Gaussovih funkcija

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Koristeći funkciju generatrise Hermiteovih polinoma dana je veza Slaterovih i Gaussovih funkcija. Ovu vezu formalno možemo interpretirati kao inverznu transformaciji integrala po Shavittu i Karplusu.

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