New Aspects in the Calculation of Electronic Momentum Properties; an All-Quantum Study

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The electronic properties of the C_6H_6 and C_6D_6 molecules have been studied by an all-quantum approach, where the classical and quantum degrees of freedom of the nuclei are taken into account in the evaluation of electronic expectation values. In the all-quantum approach suggested a Feynman path integral Monte Carlo (PIMC) formalism has been linked to an electronic *ab initio* Hamiltonian. The electronic expectation values have been calculated as averages over the manifold of nuclear configurations populated in thermal equilibrium. This theoretical setup leads to electronic expectation values that depend on the temperature and on the mass of the nuclei. The ensemble averaged electronic properties differ sizeably from the results derived on the basis of a single nuclear configuration of minimum energy. This behaviour should have physical implications for the theoretical calculation of electronic momentum properties such as Compton profiles, reciprocal form factors, etc. We describe an error source in the theoretical determination of electronic momentum properties which has not been commented so far.

Key words: Quantum Properties of Nuclei and Electrons; Path-Integral Simulations; *ab initio* Calculations; Electronic Momentum Properties; Finite-Temperature and Isotope Effects.

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