

## THURSDAY MORNING

of a Many-Body Perturbation Theory (MBPT) calculation using the computer algebra system Mathematica is presented. Wick's theorem is used to symbolically obtain the expressions corresponding to Feynman (or Goldstone) diagrams, typically determined by hand, to third order. The angular factors which arise in the atomic many-body problem, and which are also typically obtained diagrammatically, are calculated using a symbolic Fortran program and automatically linked via Math-Link to the Wick's theorem program. Complete and error-free terms are therefore efficiently obtained for potentially an arbitrary number of particles and holes. These terms are automatically numerically evaluated using externally running Fortran and C programs and a previously generated basis set to provide energies through third order and wavefunctions through second order. The terms are also printed in L<sup>A</sup>T<sub>E</sub>X form and the appropriate Feynman diagrams illustrated for ease of comparison with previous results. Application to the 1-particle, 1-hole case, as an example which illustrates the power of this approach, is given.

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**High-Precision Bethe Logarithms for Low-lying S-states of Helium** J.D. MORGAN III, J.D. BAKER, *U. of Delaware*, R.C. FORREY, *ITAMP*, M. JEZIORSKA, *U. of Warsaw* — Using a generalization of a method developed by Charles Schwartz,<sup>1</sup> we have obtained for the  $1^1S$  and the  $2^1S$  states of the helium atom highly accurate Bethe logarithms, which enter into the  $O(\alpha^3)$  Rydberg QED corrections to the energy levels. We shall describe how we obtained our results and shall compare them against the best available experimental measurements by groups at Yale<sup>2</sup> and at NIST.<sup>3</sup> This comparison illustrates the pressing need to evaluate fully the  $O(\alpha^4)$  Rydberg QED corrections, which in light of advances in the calculations of the Bethe logarithms by us and of the  $O(\alpha^4 \ln \alpha)$  Rydberg corrections by Drake, Khriplovich *et al.*<sup>4</sup> are now the leading cause of uncertainty in the theoretical estimates.<sup>5</sup>

<sup>1</sup>C. Schwartz, *Phys. Rev.* **123**, 1700 (1961).

<sup>2</sup>W. Lichten, D. Shiner, and Z.-X. Zhou, *Phys. Rev. A* **43**, 1663 (1991).

<sup>3</sup>C. J. Sansonetti and J. D. Gillaspay, *Phys. Rev. A* **45**, 1 (1992).

<sup>4</sup>G. W. F. Drake, I. B. Khriplovich, A. I. Milstein, and A. S. Yelkhovskiy, *Phys. Rev. A* **48**, R15 + 4804 (E) (1994).

<sup>5</sup>Supported by a NIST Precision Measurement Grant, NSF grants PHY-8608155 and PHY-9215442, and by an NSF grant for the ITAMP at the Harvard-Smithsonian Center for Astrophysics.

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**Laser Photoacoustic Spectroscopy Study on the Torsional-Rotational Structure of Ethanol Adsorbates on Silver Surface.** Z Y WANG, C F NG, P K LIM, H W LEUNG, W H FEI, S C CHEN, *Dept. of Physics, Hong Kong Baptist University*. — Laser photoacoustic spectroscopy (LPAS) and thermal desorption spectroscopy (TDS) were employed to study the vibrational spectrum of ethanol molecules adsorbed on polycrystalline silver surface at 108 K. In this study the strength of the bonding between adsorbate and the surface was found to be between the physisorption and chemisorption as indicated by the values of heat of adsorption measured in the TDS (33.2 kJ mol<sup>-1</sup>, 38.8 kJ mol<sup>-1</sup>, 39.5 kJ mol<sup>-1</sup>, and 44.2 kJ mol<sup>-1</sup>). Of more interest was the appearance of fine spectral structure of ethanol adsorbates on the LPAS vibrational spectrum by carbon dioxide laser. Comparing with the Fourier transform infra-red spectroscopy of ethanol molecules of gas phase in the same spectral region, we attribute our observation in LPAS that such fine spectral structure of ethanol adsorbates is to be arisen from the internal torsional-rotation of the ethanol adsorbate on silver surface. Our findings therefore show that torsional-rotational structure exists not only in free molecules in gas phase, but also in adsorbate phase. The uhv LPAS setup used in this experiment is unique. It shows that a 1 cm<sup>-1</sup> spectral resolution and 1 L sensitivity could be reached in the same time. The torsional-rotational spectral structure could be found just due to the 1 cm<sup>-1</sup> fine resolution. The uhv LPAS setup has the potential in studying other systems as well.

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### Supplementary Paper

**Time-Resolved Emission Spectroscopy of the Alkoxy Radicals** PRABHAKAR MISRA, *Howard University* — The alkoxy (RO; R = CH<sub>3</sub>, C<sub>2</sub>H<sub>5</sub>, i-C<sub>3</sub>H<sub>7</sub>) radicals play significant roles as oxidation intermediates in the combustion of hydrocarbons and in atmospheric pollution. Excimer laser radiation (50 mJ pulse @ 248 nm) was employed to photolyze RONO to produce the RO radicals in situ in a supersonic jet expansion. Tunable radiation from a Nd:YAG-pumped dye laser, frequency-doubled to generate near-UV wavelengths (of typical pulse energy 100 μJ), was used to excite the radicals. A photomultiplier tube was then employed to detect the fluorescence emission following laser excitation, and the corresponding decay curve displayed on the screen of a digital oscilloscope. Lifetime measurements involving various quanta of the CO-stretch vibration ( $\nu' = 0 - 5$ ) for CH<sub>3</sub>O, C<sub>2</sub>H<sub>5</sub>O and i-C<sub>3</sub>H<sub>7</sub>O, covered the range 0.15-3.0 μs. Significant non-radiative decay routes were found for the excited states of these RO radicals.

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