Theoretical estimation of scattering loss rates in Cold-Atom traps for novel Ultra-High-Vacuum sensors

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A new pressure sensor for Ultra-High-Vacuum (UHV) has been built at the National Institute of Science and Technology (NIST)[1]. The development of these devices relies on ensembles of trapped and laser-cooled $^7Li(^2S)$ or $^{87}Rb(^2S)$ atoms at tens of micro-Kelvin temperature. The sensors will allow measurements of extremely low UHV pressures, for which current pressure sensors based on a hot wire are not reliable. Trapped cold atoms encounter residual room-temperature atomic and molecular gases in the vacuum system, which result in cold atom losses with near 100 % efficiency. One needs accurate knowledge of collisional rate coefficients to convert measured cold-atom loss rates into measurements of pressure. We present recent results[2] of quantum scattering calculations using high-quality *ab-initio* potentials computed with the current gold-standard coupled-cluster method. We find temperature-dependent elastic rate coefficients between cold atomic $^7Li/^{87}Rb$ and room-temperature noble gases and molecular nitrogen and hydrogen. We also describe initial efforts on extending our calculations to $CO(^1\Sigma^+)$, $O_2(^3\Sigma_g^-)$ and also polyatomic molecules such as $CO_2(^1\Sigma^+)$. Scattering calculations are performed by solving quantum close-coupling equations for all collision energies necessary to converge thermalized rate coefficients for temperatures up to room temperature. The computed loss-rates can be compared to experimental results obtained at NIST. We also estimate the uncertainties of the elastic rate coefficients associated with the uncertainty in the *ab-initio* potentials and due to omitted relativistic effects.

[1] L. Ehinger, B. Acharya,D. S. Barker, J. A. Fedchak *et al*. https://arxiv.org/pdf/2204.03705.pdf
[2] J. Kłos and E. Tiesinga, J. Chem. Phys. (2022); https://doi.org/10.1063/5.0124062