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‘QUANTUM-BASED REALIZATIONS OF THE PASCAL’ STATUS AND PROGRESS OF THE EMPIR-PROJECT: QUANTUMPASCAL

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Abstract:

The QuantumPascal (QP) project combines the capabilities of 12 European institutions to enable traceable pressure measurements utilizing quantum-based methods that evaluate the number density instead of force per area to target the wide pressure range between 1 Pa and 3 MPa. This article summarizes the goals and results since the project start in June 2019.

Keywords: Pascal; refractometry; ab-initio calculations; quantum-based; pressure

1. INTRODUCTION

Current realizations of the pascal rely on piston gauges (also known as pressure balances) and liquid manometers (which contain toxic mercury). They suffer from practical and environmental limitations and their performance has remained essentially unchanged in recent decades.

Thanks to the implementation of the redefined International System of Units (SI) in May 2019, in which the uncertainty of the Boltzmann constant was eliminated [1], [2], possibilities opened up for the realization of photon-based standards for pressure that are primarily limited by the accuracy of *ab-initio* quantum calculations of relevant gas parameters (molar polarizabilities and virial coefficients) [3].

The QuantumPascal (QP) project (Figure 1), pursued by several National Measurement Institutes (NMIs) together with a few selected universities, aims to develop novel quantum-based pressure standards based on optical, microwave, and dielectric methods and to assess their potential with the aim of replacing the existing mechanical based vacuum standards [4]. The new techniques have the great potential to be miniaturized, faster, and can provide calibration-free pressure measurements for industry at a fraction of the current cost in the future.

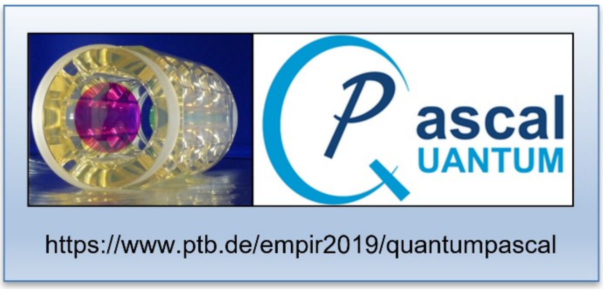

Figure 1: Logo of the QP project. It shows a Zerodur-based Fabry-Pérot resonator used for pressure assessments at CNAM.

This article summarizes the goals of the QP project, and the results obtained up to date. The specific objectives of the project are given in the Appendix. First, results are presented related to Fabry-Pérot (FP) based refractometry, which is the most common means of realising refractometry, regarding its main challenges, *viz.* pressure-induced deformations, the assessment of the temperature, and gas impurities. It also summarizes recent results concerning the gas modulation refractometry (GAMOR) methodology.

Thereafter, the current status of several alternative techniques not based on FPCs (FP-cavities) will be presented. They are Rayleigh scattering (RAY), multiple reflection interferometry (UNIT), two gas thermometry techniques namely dielectric-constant gas thermometry (DCGT) and refractive index gas thermometry (RIGT), a superconducting version of RIGT, and absorption spectroscopy of selected molecular species using very long optical paths.

Furthermore, to provide highest accuracy, sufficient knowledge about gas parameters is required. Therefore, the project also addresses quantum-based *ab-initio* calculations of static and dynamic polarizabilities, diamagnetic susceptibilities together with dielectric virial coefficients of He, Ne and Ar. Finally, work related to comparisons between the developed methods and conventional established methods is presented.

2. DESCRIPTION OF THE PROJECT

The programme comprises four technical work packages as follows, namely WP1 – WP4:

2.1. WP1: Pressure measurements based on Fabry-Pérot cavity based refractometry

WP1 addresses pressure measurements by means of FPC based refractometry. Three of the main challenges to reach the uncertainties in the low ppm (10^{-6}) level are addressed in three consecutive tasks.

The first task deals with the cavity deformation that takes place when the cavity is filled with gas. For 100 kPa of He or N_2, a relative change in cavity length of 3×10^{-11} or 3×10^{-10}, respectively, produces the same relative shift in the beat frequency as a change in gas pressure of one ppm. The aim of this task is therefore to assess the deformation of a range of FPCs and to develop means of either reducing the deformation or determining its extent (to compensate for it). After all partners independently modelled the deformation of a specific cavity, with a given geometry and material, that exists in one of the partners' laboratories [5], they each modelled a cavity they subsequently will experimentally characterize [6].

The second task is concerned with the development of methods for accurate assessment of the temperature of the gas in the FP cavity. To convert an assessed molar density to pressure, the temperature of the gas needs to be well known (an uncertainty in temperature of 300 μK corresponds to an uncertainty in pressure of 1 ppm) and should therefore also be stable. An additional reason for the latter is that a non-stable temperature also will induce thermal expansion of the cavity. This is addressed firstly by developing a means of stabilising the temperature of the cavity spacer (so as to minimising its gradients), and secondly by developing methods for absolute and traceable temperature determinations. Systems based on Pt-100s, classical thermistors, or the melting point of Ga have been developed that either use resonators made of Invar, in which there are minimal thermal gradients (see below) [7], or Zerodur, where most of the gas under investigation is in direct contact with thermalized copper surfaces [8]. Additionally, utilizing a FP spacer made from sapphire the feasibility of high-resolution photonic thermometry for temperature control will be investigated, of which the first results will be presented by Molto et al. in [9].

The third task addresses the question of gas permeation, which is of importance since it can potentially bring in impurities into the gases. This is of particular importance when a system is to be characterized with respect to its cavity deformation by use of the two-gas method of which one is He [10]. In this task, the gas diffusivities, D, with respect to He were measured for potentially suitable materials. The results show that, at $T = 23$ °C, for ULE D_{ULE} is $4.2(1) \times 10^{-8}$ cm²/s, which is 6×10^2 times larger than for Zerodur, for which D_{Z} is $7(1) \times 10^{-11}$ cm²/s. Furthermore, our results show that the corresponding He solubility for ULE is about 30 times higher, resulting in a more than four orders of magnitude lower permeability for Zerodur at room temperature than for ULE glass (soon to be reported in an upcoming article). For materials such as Invar and sapphire no permeation of gas has been found, for the latter not even above 400 °C.

As **a fourth task**, to improve on performance in refractometry, the development of gas modulation methodologies has been addressed. The GAMOR methodology, which is based upon a periodical modulation of the gas in the measurement cavity, has demonstrated an extraordinary ability to reduce the influence of disturbances in refractometry systems, which implies that systems utilizing this methodology has demonstrated an outstanding precision.

It has been found that its abilities to reduce disturbances, scrutinized in detail in [11], have made it possible to realize a high-performance FP-system using a cavity spacer made of Invar [12]. This material has several appealing properties compared to commonly used glass materials, e.g., a high volumetric heat capacity, which reduces temperature fluctuations; a large thermal conductivity, which reduces thermal gradients and thereby allows for accurate temperature assessments; a high Young's modulus, which gives the cavity a low pressure induced deformation; and a low degree of He diffusivity, permeation, and solubility, which preserves gas purity. In addition, it can be machined in a standard metal workshop, whereby more complicated geometries swiftly can be created at a low cost. Utilizing a GAMOR-based Invar FP cavity system could, when assessing pressure at 4303 Pa, provide (for measurement times of 10^3 s) a minimum Allan deviation of 0.34 mPa, corresponding to a relative deviation of 0.08 ppm [12].

A potential drawback of the GAMOR methodology is that the modulation of the gas potentially can affect the temperature distribution in the cavity system by so called *pV*-work. A scrutiny of this was therefore performed. It was found that, due to the small dimensions of the Invar-based FPC system and the thermal properties of Invar, for the case with 30 kPa of N_2 being assessed, the temperature of the gas species is within 1 mK of the cavity wall in less than 1 s, that after 10 s an upper limit for the temperature increase at any point of the spacer is 1 mK, and that, at the end of the gas filling, the difference in temperature between the gas and the locations of the temperature probes in the spacer block are less than 0.3 mK [13]. A subsequent study has indicated that the actual fluctuations of the temperature are markedly less than the predicted upper limits, implying that the system has similar properties when 100 kPa of N_2 is addressed [14]. This implies that assessments made by use of the GAMOR methodology are not significantly affected by any temperature fluctuations due to the filling and evacuation of gas.

The high precision has also allowed for the realization of a disturbance-resistant methodology for assessment of cavity deformation [6]. By scrutinizing the difference between two pressures: one assessed by the uncharacterized refractometer and the other provided by an external pressure reference system, at a series of pressures of two gases with dissimilar refractivity, He and N_2, the cavity deformation could be assessed with such an accuracy that, under the condition that the impurities in the gases can be neglected, the uncertainty in the deformation contributes to the uncertainty in the assessment of pressure of N_2 with solely a fraction (13%) of the uncertainty of its molar polarizability, presently to a level of a few ppm. This implies that, as long as gas impurities can be neglected, cavity deformation is not a limiting factor in FP-based refractometer assessments of pressure of N_2 [5].

The GAMOR methodology has also, thanks to its mitigation of the influence of various types of disturbances, made it possible to construct transportable systems [15], [16], [17]. A comparison between two GAMOR-based systems has demonstrated that the systems have an extraordinarily high short time precision, in the 10^{-8} range [16].

A close scrutiny of the Invar-based system has revealed that the system is capable of assessing pressure with an extended uncertainty ($k = 2$) of $[(10\ \text{mPa})^2 + (10 \times 10^{-6} P)^2]^{1/2}$ [18], which is in pair with the so far, most accurate FP-refractometry system developed by NIST.

A procedure for *in situ* determination of the frequency penetration depth of coated mirrors in FP based refractometers, and the influence of this and the Gouy phase on the assessment of refractivity and pressure, has recently been performed. It is based on assessments of the absolute frequency of the laser and the free spectral range of the cavity. The procedure was demonstrated on the Invar-based system with high-reflection mirrors at 1.55 μm. It was found that the influence of penetration depth could be assessed with such a low uncertainty that it does not significantly contribute to the uncertainties ($k = 2$) in the assessment of refractivity ($< 8 \times 10^{-13}$) or pressure (< 0.3 mPa) when 100 kPa of N_2 is addressed [19].

The GAMOR methodology has been described in some detail in the literature [20], [21], [22].

2.2. WP2: Alternative non Fabry-Pérot based approaches for the realisation of absolute and partial pressure standards

In WP2, the feasibility of using alternative techniques to assess either temperature, molar density, or pressure is investigated, specifically RAY, UINT, DCGT, RIGT, and TDLAS. Jointly, they cover the pressure range from 1 Pa to 3 MPa.

The first task is devoted to a Rayleigh scattering-based system (RAY) for pressure measurements up to 1 MPa. A precondition for the realization of RAY was a series of optical simulations conducted to optimize the design including a multi-step stray light analysis. Upgrading the simulated system with specific optomechanical components revealed a reduction factor better than 1×10^{-5}, which fully meets the requirements. The optical layout has been consequently realized to minimize stray light effects.

The RAY setup was fully making use of Al-based vacuum technology equipped with a temperature control and measurement unit hosting up to six temperature sensors. The system is currently based on a blue laser source and a cooled camera detector which measures the light scattered by the gas molecules as a function of density or pressure.

A custom software, written in Python, has been developed to analyse the acquired images from the camera detector, with the dual purpose of detecting and correcting effects caused by eventual spurious scattering centres and calculating the intensity of scattered light. The realized software and the design of the RAY system were presented in [23].

After a preliminary result up to 400 kPa, exhibiting a strong linear dependence between pressure and scattered light, the system has been recently tested up to 1 MPa in nitrogen. This extension of the assessed range led to a correlation between pressure and scattered light that could be excellently fitted with a quadratic polynomial ($R^2 \geq 0.999999$). This behaviour is plausible since the density virial expansion for N_2 only needs to include up to the second order coefficient without significant loss of accuracy. Metrological characterizations and measurements with Ar and He are ongoing testing the ability of RAY to perform direct comparisons of the molar polarizabilities of different gases.

The second task deals with an optical pressure standard using an unbalanced interferometric technique (UINT). This multi-reflection technique aims to propose an alternative route especially at barometric pressures and was used in the 100 Pa – 100 kPa range, with a targeted uncertainty of 10 ppm at 100 kPa. The UINT realization has benefitted from a series of optical simulations, essential for the final design. Since the optical path inside the double mirror assembly of UINT, i.e., the measurement arm of the interferometer, is crucial and influenced by pressure induced deformations, the optical layout has been realized considering the output of the FEM simulations performed in WP1 combined with ray tracing studies. To estimate the value of nominal optical path, Gaussian beam propagation was used to predict the value of misalignment between the entering and the exiting laser beam. An independent experiment revealed an optical path length of the unbalance that agreed with the simulations and allows to meet the expected target uncertainty.

To overcome the challenge for a primary photonic realization, the UINT system has been placed in a specially designed Al based UHV chamber inside an Al box to realize a double staged temperature control at the mK level.

The UINT recently demonstrated an ability of assessing barometric pressure with an uncertainty of 10 ppm, improved by an order of magnitude as compared to previous achievements [23], [24], [25]. The UINT pressure standard has been also compared to a reference pressure standard, a barometer, in the 70-100 kPa range: the results show a relative difference of ± 20 ppm for N_2, fully covered by the related uncertainties. A manuscript describing the new UINT system is under preparation.

In task 3, pressure standards based on the polarizing gas thermometry methods DCGT and RIGT are developed for the pressure range 1 MPa to 3 MPa. RIGT techniques exploit the high accuracy which achievable by measuring resonance frequencies of microwave modes excited, in the GHz range, within gas-filled resonators with internal dimension of a few centimetres. The current development aims to reduce the uncertainty of this technique below 5 ppm. In DCGT, the particle density of the measuring gas is assessed via determination of the dielectric-constant from the relative change of capacitance of a measuring capacitor and utilization of the Clausius-Mosotti equation. Gaiser *et al.* have recently demonstrated that the principle can be used to realize a primary pressure standard with He [26]. Due to the low uncertainties of the corresponding gas properties, which were calculated by *ab-initio* quantum calculations, relative uncertainties of 5 ppm were reached for pressures up to 7 MPa. However, the utilization of a custom-built capacitance bridge was required due to the low measuring effect. In this project the capabilities of a much smaller setup and commercially available measuring equipment are presently explored. To reach competitive uncertainties, Ar is used as a measuring gas since its molar polarizability is a factor of eight higher compared to He. This dielectric gas pressure standard is currently compared to a conventional pressure standard.

In task 4, a superconductive RIGT was realized utilizing a microwave cavity made of copper with internal Nb coating and used at room temperature and at temperatures below 10 K.

The performance was also tested with He and Ar at 90 K, in the pressure range between 200 Pa and 20 kPa. A detailed description can be found in the Thesis of Gambette [27].

The last task addresses a partial pressure standard utilizing absorption spectroscopy. To perform high precision TDLAS measurements, one must consider the laser linewidth and its effect on the assessed absorbance. It was evaluated that for a target uncertainty of 500 ppm the laser linewidth must not exceed 10^{-9} µm when absorption measurements on CO_2 in the MIR region are performed. The linewidth narrowing of the utilized QCLs was achieved experimentally by locking the lasers to a tuneable FPC. Additionally, absorption line strength measurements of H_2O were carried out at 23 °C at a wavelength of 937 nm and published in comparison with theoretical calculations by Rubin et al. [28]. The updated values for the experimentally assessed line-intensity is $S(293K) = 3.076 \times 10^{-22}$ cm/molecule with an uncertainty of 0.7% in excellent agreement with the recent theoretical results.

2.3. WP3: Theoretical values of the thermodynamic and electromagnetic properties of He, Ne and Ar, the electromagnetic properties of CO and CO_2 and experimental checks

A prerequisite for the refractivity-based pressure standards to be primary methods is the exact knowledge of the polarizabilities (static or dynamic, depending on the technique used) and the lower orders of dielectric and density virial coefficients of the atomic or molecular gas addressed. For the simplest gas species, they can be obtained from *ab-initio* calculations.

The first two tasks address the static (task 1) and dynamic (task 2) properties of the noble gases He, Ne and Ar, where the lowest uncertainties were achieved for He. Puchalski *et al.* determined the static value of the polarizability of He with a relative uncertainty of 1×10^{-7} which is over one order of magnitude lower than the most precise experimental determination by Gaiser *et al.* [29], [30]. To obtain the dynamic polarizabilities required for optical experiments, it is recommended that the dispersion published by Puchalski *et al.* in 2016 should be utilized [31]. For the static polarizability of neon, the lowest uncertainty, ca. 2 ppm, was reached experimentally by Gaiser *et al.* [30], which is one order of magnitude lower than the so far best theoretical determination by Hellmann (QP collaborator) [32]. To utilize the highly precise experimental static value for optical experiments, the required dispersion was calculated by Lesiuk *et al.* together with the magnetic susceptibility [33]. Furthermore, the dielectric virial coefficients are required. Garberoglio *et al.* have developed a path-integral approach to calculate the second [34] and third [35] static and dynamic virial coefficients of He, Ne, and Ar based on the best available literature potentials and polarizabilities. Improved pair polarizabilities and, in case of He, the three-body polarizability tensor, which were developed within the frame of this project, are currently used to refine these results. The results of Garberoglio and Harvey for the second dielectric virials were confirmed by Song (QP collaborator) and Luo using a different method for computation [36]. Experimentally, the results for He were checked by highly precise DCGT experiments by Gaiser and Fellmuth [37]. For Ne, the evaluation of the experimental data is under progress. In case of Ar first experimental values for the second dielectric virial coefficient were obtained by Günz [38]. Theoretical work on Ar is overall challenging due to the more complex atomic structure and, thus, at this point, part of ongoing research.

2.4. WP4: Comparison of new and improved pressure standards and methods with established methods

To validate the developed instrumentation, WP4 includes a comparison of all the novel methods with the primary standards (assessing force per area) which are available at the different NMIs.

Task 1 is about the comparison of conventional primary pressure standards to the novel methods. Many of them will take place at the end of the project but preliminary works have been performed at PTB and INRiM (calibration of the piston cylinder assembly used for RIGT at INRiM) and at RISE for the preparation of the circular comparison.

Task 2 addresses a circular comparison using RISE’s transportable optical FP-based refractometer. Although it was designed and realized in time, the Covid-19 pandemic gave rise to significantly delays of this activity. The refractometer has by now been engaged in a ring comparison at different institutes in Sweden, Germany, Italy, and France.

Regarding the robustness and transportability, it can be concluded that while the refractometer had often been exposed to rough handling by “general transporting companies”, it has so far always arrived in such a good shape that measurements could be initiated. Details about this measurement campaign will be presented in an additional publication by Forssén *et al.* in [17].

3. SUMMARY AND CONCLUSION

This paper presents an overview of the current status of the QuantumPascal project which started in June 2019 and will be completed in November 2022.

The overall aim of the project is to develop novel quantum-based pressure standards based on optical, microwave, and dielectric methods and to assess their potential with the aim of replacing existing mechanical based pressure standards. It takes advantage of recent advances in various measurement techniques, combined with the outstanding progress of quantum-based calculations of gas properties, to develop novel, improved pressure standards.

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5. APPENDIX

The specific objectives of this project are:

Obj. 1: To improve on the accuracy and extend the working range of quantum-based FP refractometry methods that have the potential to become primary standards of the SI unit of pressure, the pascal. The target uncertainties (k = 1) and pressure ranges are 500 ppm in the range 1 Pa - 1 kPa and 10 ppm in the range 1 kPa - 100 kPa.

Obj. 2: To improve on the accuracy and evaluate the potential of alternative (non FP based) quantum-based approaches and detection methodologies for the realisation of absolute and partial pressure standards, including superconductive microwave resonators, Rayleigh scattering, multi reflection interferometry, gas thermometry methods, absorption spectroscopy of selected molecular species with very long optical pathways with target uncertainties (k = 1) less than 500 ppm between 1 Pa and 10 Pa, less than 50 ppm between 1 kPa and 100 kPa, less than 500 ppm between 100 kPa and 1 MPa and less than 5 ppm between 1 MPa and 3 MPa, depending on the measurement technique.

Obj. 3: To develop improved ab-initio calculations of the thermodynamic and electromagnetic properties (static and dynamic polarisability, diamagnetic susceptibility along with dielectric- and density virial coefficients) of He, Ne, and Ar and the electromagnetic properties (intensities of specific absorption lines) for CO and CO_2 of gases as needed to meet the objectives above. For gases other than He, the accuracy of the calculations (targeted uncertainty contributions of 1 ppm to 5 ppm at 100 kPa) are to be validated by comparisons with results from experiments using He as a calibrating reference substance.

Obj. 4: To demonstrate the performance of the methods developed in the objectives above by comparison with conventional primary absolute pressure standards such as pressure balances.

Obj. 5: An additional aim is to facilitate the take-up of the technology developed in the project by end users, i.e., the scientific, metrological, and industrial communities and standards developing organisations.